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SUBJECT: Derivation of Health-Based Environmental Screening Levels (HBESL) for  
Chemical Warfare Agents

The enclosed report provides technical guidance regarding investigations of environmental media potentially contaminated with chemical warfare agent. Ongoing reviews of associated scientific literature and research may require future updates and/or reevaluation of the information. However, the document presents the state of the science and establishes the current Army standard practice to such investigations. The approach includes the application of specified risk assessment models along with stakeholder participation and the consideration of identified areas of uncertainty.

This information has been reviewed and received the concurrence of the organizations represented on the DA Steering Committee for Standards for Emergency Response, Remediation, Restoration, and Demilitarization of Chemical Warfare Materiel. The report should be distributed to the field for immediate use.

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# **DERIVATION OF HEALTH-BASED ENVIRONMENTAL SCREENING LEVELS FOR CHEMICAL WARFARE AGENTS**

A Technical Evaluation

March 1999

*Prepared by*

**U.S. ARMY CENTER FOR HEALTH PROMOTION  
AND PREVENTIVE MEDICINE**  
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*in conjunction with*

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**LOCKHEED MARTIN ENERGY RESEARCH CORP.**  
for the  
**U.S. DEPARTMENT OF ENERGY**  
under contract DE-AC05-96OR22464

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## EXECUTIVE SUMMARY

### DERIVATION OF HEALTH-BASED ENVIRONMENTAL SCREENING LEVELS FOR CHEMICAL WARFARE AGENTS

#### 1. PURPOSE.

The purpose of this document is to evaluate currently available data and scientific methods for the assessment of potential chronic human health risks from residual chemical warfare agents in environmental media. With the identified information, associated health-based environmental screening levels (HBESLs) are then calculated. Specifically, existing U.S. Environmental Protection Agency (USEPA) chronic risk assessment methods are used with parameter assumptions defined for two common theoretical exposure scenarios to calculate a set of HBESLs for soil for the vesicant chemical warfare agents sulfur mustard (HD) and Lewisite, and the nerve agents Tabun (GA), Sarin (GB), Soman (GD) and VX. *The document is a technical reference reflecting the scientific models and data available at the time of publication. The user is cautioned to consider any scientific advances that may impact the information contained herein.*

#### 2. APPLICATION AND LIMITATIONS.

2.1 Environmental screening levels (referred to by different names by different USEPA Regions) are low-level concentrations of individual chemicals in environmental media which, if not exceeded, are unlikely to present a human health hazard for specific exposure scenarios. Different EPA regions have used risk assessment models to establish screening levels for hundreds of industrial and agricultural chemicals that present contamination problems, and similarly, these models may be used to calculate screening levels for chemical warfare agents. During the initial evaluation phase of an environmental health risk assessment, these pre-established environmental screening levels for chemical compounds can aid the assessment process by their use as 'action or no-action' determinant criteria. For a specified scenario, if the actual soil concentrations fall below an established screening level, typically no further 'action' is deemed necessary. If concentrations are above the screening level, additional 'action' is generally required. This 'action' requirement may be met by a variety of procedures to include: performing a detailed site-specific health risk assessment; applying management controls to minimize exposure; implementing treatment/remedial operations; or a combination of these options. By focusing assessment efforts only where "action" is necessary, screening levels can help to optimize resources and minimize unnecessary expenditures of time and money. Screening levels, however, may not be appropriate for all situations. First, certain technical assumption criteria must be met, and second, all stakeholders (including specific Army activities/installations, state/local regulators, and the public) must agree to their appropriateness. *The calculated screening levels in this document are supported with the necessary documented scientific rationale; however, site-specific stakeholder input is a necessary part of their use.*

2.2 Another benefit of environmental screening levels is that they allow a means to determine whether analytical detection capabilities for chemical contaminants are adequate. This is particularly beneficial if the compounds are very toxic and the resulting screening levels are extremely low.

2.3 Finally, in addition to the utility of the screening levels, this document provides a consolidated reference for discussion/documentation of various exposure parameters and chemical-specific environmental fate issues. *Much of the information regarding the use of a particular risk assessment model and certain input parameters can be used to facilitate site-specific risk assessments.*

### 3. SCOPE.

3.1 This report compares and discusses the differences and limitations of three USEPA risk assessment methods. These are the USEPA Region III Risk-Based Concentration (RBC) model, the USEPA Region IX Preliminary Remediation Goal (PRG) model, and the recently established USEPA Office of Solid Waste and Emergency Response Soil Screening Level (SSL) model. Using these methods and the Army-approved interim chronic toxicity values<sup>1</sup> for the chemical agents, this report calculates HBESLs for two common generic exposure scenarios (residential and commercial/industrial) that are used by the EPA and which may be used to meet screening goals for cleanups conducted at DOD/Army facilities/sites. These HBESLs address the long-term/chronic exposures to residual levels of chemical agent in the environment at such sites and are not applicable to deployed troops or acute exposures created by catastrophic chemical agent releases. Considerations regarding the potential application of chronic risk models to other scenarios, including problems with such applications, are evaluated in various appendices of this document (See appendices C and D).

3.2 Descriptions of agent HBESLs include documentation of efforts to make the most reasonable assumptions for the exposure parameters and relevant pathways associated with the residential and industrial/commercial exposure scenarios. USEPA default values are used for many of the population-, chemical-, and site-specific parameters. However, factors such as agent persistence, degradation, and dose-response relationships were carefully analyzed and non-default values incorporated into the HBESL derivation procedures. In the process of evaluating agent environmental fate and transport, the key environmental breakdown products of chemical agents were identified. Specific discussion regarding the potential for chemical agent contamination of ground water and drinking water is also presented in this document.

### 4. CONCLUSIONS.

4.1 The three EPA methods assessed are very similar; the differences do not generally yield substantially different screening levels. The additive pathway approach represented by PRG's generally results in some of the more conservative (lower) values, primarily due to the additive effects of the inhalation route, and, to some degree, the dermal route. The SSL inhalation pathway model also produces some of the most conservative values. For the vesicants HD and L, the RBC model must be used cautiously to ensure resulting concentrations do not yield acute effects. In all, the "best" model may vary for different chemicals and situations. The benefits and disadvantages of one method over another are somewhat speculative, but depend

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<sup>1</sup> The chronic toxicity values [reference doses (RfDs)] associated with the agents are identified as "interim" by the Army and are undergoing review and evaluation by external expert panels. If the chronic toxicity values are modified as a result of this review process, the calculated HBESLs in this report may be subject to change. (DA 1996a)

on chemical and site/exposure-specific considerations. Ultimately, stakeholders (including site regulators, the public, and Army personnel) must evaluate the available information to determine whether the use of a screening approach is warranted and, if so, what models and parameters best suit the situation.

4.2 The HBESL values calculated in this document are intended to represent conservative values for use in *screening* contaminated sites for potential human health risks. The degree of ‘conservatism’ that is truly represented cannot be quantified due to the uncertainties inherent to the risk assessment models. These uncertainties are further compounded by limited data regarding both the chemical warfare agents and the human exposure process. A limitation of the application of the HBESLs for generic scenarios is that, by using a standardized approach and assumptions, unique site-specific variables may be overlooked. Therefore, before application of HBESLs as action/no-action determinants, the user must first evaluate the situation to ensure that certain assumption criteria are met. This includes ensuring that all stakeholders have input to the application of screening levels. However, despite the weaknesses associated with deriving and applying HBESLs, they provide a mechanism to make efficient, consistent, and scientifically-based action/no-action decisions when assessing the potential for chronic health effects to exposed populations.

4.3 While chemical agent residue could potentially exist in the environment for extended periods of time, it is a realistic possibility that the agents themselves will degrade/breakdown relatively rapidly. Current EPA models do not consider environmental degradation; it is therefore quite possible that actual exposure durations/frequencies are significantly overestimated resulting in conservatively ‘safe’ screening levels. *With the exception of HD, which under certain environmental conditions could persist for particularly extended periods of time agent after being encapsulated in an inert polymeric coating formed by its hydrolysis products, the other chemical agents described in this report would generally never persist more than a few months.* The complex issue of degradation should be considered in chemical and site-specific evaluations when using screening levels and may need to be more critically incorporated in a site-specific risk assessment. The issue of degradation, however, goes beyond the persistence of the agents themselves. In the cases of Lewisite and VX, assessments for the presence of breakdown compounds Lewisite oxide and inorganic arsenic (for Lewisite) and S-(Diisopropylaminoethyl) methylphosphonothioate (i.e. EA-2192, for VX) are warranted due to their particular toxicity and potentially significant persistence. Other likely breakdown products such as thiodiglycol from HD, and methylphosphonic acid (MPA) from the G-agents and VX, do not pose a significant health risk. However, due to their persistence in the environment, they may be useful indicators of historical chemical warfare agent presence.

4.4 It is unlikely that the chemical agents addressed in this document will contaminate ground water. Site-specific evaluations are recommended to identify those potential circumstances where potential ground-water contamination should be evaluated. It is also unlikely that these agents would contaminate a drinking water source. Site-specific assessment should be conducted only for those circumstances where contamination of a drinking water source is a realistic concern.

4.5 Other applications of these models may be an appropriate mechanism to assess other scenarios where there is potential for long-term or repeated exposures (such as for waste management or when assessing impervious contaminated surfaces). For these potential applications of chronic risk assessment models, common generic assumptions do not currently exist. Evaluating risks in these scenarios is the subject of potential future initiatives.

## 5. RECOMMENDATIONS.

The Table below lists HBESL values for two common generic scenarios using three current EPA chronic risk assessment methodologies, common default parameters, and chemical-specific parameters. The information in this document can be used to assist site-specific stakeholders in determining if screening levels can be used, and if so, what models and parameters best fit unique situation needs. The HBESLs can be used as action/no-action determinants ('action' meaning to perform site-specific health risk assessment; apply management controls; treat/remediate; or a combination of these) when assessing the potential for chronic health effects to exposed populations so long as the following conditions are met:

5.1 *Levels of risk are acceptable to the situation (see Section 1.3.2).*

5.2 *Assumptions made in these scenarios are at least equally conservative, if not more conservative, than site-specific values.*

5.3 *Substance concentrations and exposure assumptions are not expected to be acutely toxic (see Section 1.3.8)*

5.4 *A single chemical is of concern (see Section 1.3.9).*

5.5 *Ground-water contamination is not considered to be a concern (see Appendix E).*

5.6 *Risk to ecological receptors is not expected (see Section 1.3.10).*

<b>Table Exec-1: Range of Estimated HBESL Values for Chemical Warfare Agents</b>						
	Residential soil (mg/kg)			Industrial soil (mg/kg)		
	RBCs	PRGs	SSLs	RBCs	PRGs	SSLs
<b>HD</b>	0.55	0.01 <sup>a</sup>	0.016	14	0.3 <sup>b</sup>	NA
<b>Lewisite<sup>d</sup></b>	7.8	0.3	7.8	(7.8) <sup>e</sup>	3.7	NA
<b>GA</b>	3.1	2.8	1.2	82	68	NA
<b>GB</b>	1.6	1.3	0.5	41	32	NA
<b>GD</b>	0.31	0.22	0.31	8.2	5.2	NA
<b>VX<sup>c</sup></b>	0.047	0.042	0.047	1.2	1.1	NA

<sup>a</sup> Cancer-based; calculated for a target risk level of 10<sup>-5</sup>

<sup>b</sup> Cancer-based; calculated for a target risk level of 10<sup>-4</sup>

<sup>c</sup> Assessment should include EA-2192, a particularly toxic and relatively persistent breakdown component of VX. Due to similar toxicity, the HBESLs derived for VX can be used for EA-2192.

<sup>d</sup> Assessment should include CVA, Lewisite oxide, and arsenic, three persistent breakdown products of Lewisite. USEPA screening levels for inorganic arsenic should be consulted. HBESLs for Lewisite can be used for Lewisite oxide.

<sup>e</sup> RBC value derived for the commercial/industrial scenario was potentially above acute toxicity levels, therefore the upper bound value of the residential scenario is suggested as a substitute.

## 1. INTRODUCTION

### 1.1 PURPOSE

The purpose of this document is to evaluate currently available data and scientific methods to assess the potential chronic human health risks from residual chemical warfare agents in environmental media. With the identified information, associated health-based environmental screening levels (HBESLs) are then calculated. Specifically, existing EPA chronic risk assessment methods are identified and then used with parameter assumptions for two common theoretical exposure scenarios to calculate a set of HBESLs for soil for the vesicant chemical warfare agents sulfur mustard (HD), Lewisite, and the nerve agents Tabun (GA), Sarin (GB), Soman (GD) and VX. *The document is a technical reference reflecting the general scientific models, assumptions, and data available at the time of publication. The user is cautioned to consider both site specific information as well as any scientific advances that may impact the values contained here or their application.*

#### 1.1.1 Scope

Specifically, this report compares and discusses the differences and limitations of three U.S. Environmental Protection Agency (USEPA) risk assessment methods. These are the USEPA Region III Risk-Based Concentration (RBC) model, the USEPA Region IX Preliminary Remediation Goal (PRG) model, and the recently established USEPA Office of Solid Waste and Emergency Response (OSWER) Soil Screening Level (SSL) model. Using these methods and the Army-approved interim chronic toxicity values for the chemical agents, HBESLs for the vesicant chemical warfare agents Lewisite and HD, and the nerve agents GA, GB, GD and VX were calculated. Specifically, this document includes HBESLs for soil for two common, generic exposure scenarios: the residential scenario and the commercial/industrial. These same two scenarios are used by the EPA to establish screening levels for hundreds of industrial and agricultural chemicals. These screening levels provide for a process of a first-phase, preliminary evaluation of contaminated sites by means of identifying contaminants of concern and determining if additional evaluation is warranted<sup>1</sup>.

Similarly, these HBESLs address the long-term/chronic exposures to residual levels of chemical warfare agent materials in the environment at potential Army environmental restoration and Formerly Used Defense (FUD) sites. In addition, potential applications and limitations of the use of these chronic risk assessment models for scenarios involving less common assumptions are discussed. In any application, there are limitations to the usefulness of these models and, in certain cases, the standard assumptions and/or the models themselves are not appropriate. Specific examples of such limitations are described.

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<sup>1</sup>Note: As described in more detail in sections 1.1.2 and 1.2.2, screening levels should not be construed as cleanup levels.

### 1.1.2 Application

During the initial evaluation phase of an environmental health risk assessment, pre-established environmental screening levels for chemical compounds can aid the assessment process by their use as “action or no-action” determinant criteria. For a specified type of scenario, if the actual soil concentrations were to fall below an established screening level, no further “action” would be deemed necessary. If concentrations were above the designated screening level, additional “action” would be necessary. This “action” requirement may be met by a variety of options to include: performing a detailed site-specific health risk assessment; applying management controls to minimize exposure; implementing treatment/remedial operations; or a combination of these options. By focusing assessment efforts in this manner, screening levels can help to optimize resources and minimize unnecessary expenditures of time and money. Screening levels, however, may not be appropriate for all situations. First, certain technical assumption criteria must be met, and second, all stakeholders (e.g. state/local regulators, public and Army personnel ) must agree to their appropriateness. *Given the current scientific methodology and information available, the calculated values in this document represent reasonable screening level values; however, their use requires both an understanding of the associated uncertainties and data gaps as well as site-specific stakeholder input.*

Another benefit of pre-established environmental screening levels is that they provide a means to determine whether analytical detection capabilities for chemical contaminants are adequate. This is particularly beneficial if the compounds are very toxic and the resulting screening levels are extremely low.

Finally, in addition to the utility of the pre-established screening levels established in this document, much of the information regarding the selected risk assessment model and input parameters can be used to facilitate the *site-specific* risk assessments. This document provides a consolidated reference for discussion/documentation of various exposure parameters and chemical-specific environmental fate issues.

## 1.2 BACKGROUND

### 1.2.1 General USEPA Risk Assessment Methodology

The scientifically accepted method of assessing potential health risks from contaminated environmental media is based on the algorithm models designed and standardized by the USEPA for assessing risks at Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) sites, also known as “Superfund” sites. The “health risks” potentially associated with such sites are independently assessed for noncarcinogenic (or “noncancer”) and carcinogenic (cancer) endpoints. Noncancer risks are determined by comparing estimates of exposure to noncancer-causing chemical contaminants for multiple exposure pathways (e.g., ingestion, inhalation, and dermal contact and absorption) with toxicity values independently derived from laboratory or epidemiological data [Risk Assessment Guidance for Superfund (RAGS), USEPA, 1989b]. Noncancer toxicity values consist of oral reference doses (RfDs) and inhalation reference concentrations (RfCs). An RfD is “an estimate (with an uncertainty spanning

perhaps an order of magnitude or greater) of a daily (ingestion) exposure level for the human population, including sensitive subpopulations, that is likely to be without an appreciable risk of deleterious effects during a lifetime" (USEPA, 1989). Likewise, an RfC is an air concentration of a chemical that is not expected to produce any deleterious effects even if (inhalation) exposures continued for a lifetime (USEPA, 1994b). Excess cancer risks at a Superfund site are calculated from estimates of potential exposure and from cancer slope factors (CSFs). A CSF defines the upper bound lifetime probability of an individual developing cancer as a result of being exposed to a unit dose of the chemical. For industrial chemicals, RfDs, RfCs, and CSFs derived by USEPA are made available to the public by being incorporated into USEPA's Integrated Risk Information System (IRIS; USEPA, 1997a) or on the Superfund Health Effects Assessment Summary Tables (HEAST; USEPA, 1997c).

Actual site-specific risk assessments (sometimes referred to as baseline risk assessments) involve detailed, site-specific analyses of all potential pathway-specific exposures. Potential exposures across all likely pathways for a given chemical are summed. For noncancer endpoints, the total exposure is converted into a daily dose and compared to the chemical's RfD. For cancer endpoints, the total cancer risk associated with the daily exposure is determined using the chemical's CSF. *A baseline risk assessment incorporates as much site-specific information as possible to adequately define the likely exposure pathways, and includes such factors as current and expected uses of the site, population demographics, soil type, and environmental fate and transport analyses to assess the potential for offsite migration of the contaminants. Baseline risk assessments generally require significant time and effort to collect and validate site-specific data. They are often conducted at a site where initial screening has indicated a potential risk concern before remedial options are considered.*

### 1.2.2 Screening Approaches

In conducting health risk assessments at Superfund sites, a tiered approach is used in which the first step is a screening evaluation where the measured levels of environmental contamination are compared with pre-established environmental screening levels. Environmental screening levels (referred to by different names by the various USEPA Regions) are low-level concentrations of individual chemicals in environmental media, which, if not exceeded, are unlikely to present a human health hazard for specific exposure scenarios. These "low-level" concentrations are back-calculated from the USEPA risk assessment models using predetermined, conservative "acceptable risk" quantifiers. The screening approach can aid the risk assessment process by identifying those sites where either a more detailed baseline risk assessment or some other form of action (such as remediation) is necessary. However, the screening process and pre-established screening level lists vary. The screening evaluation and the final screening values are a function of the number of environmental media and exposure pathways that are included. Screening methods based on multi-media and multi-pathway analyses are intrinsically more conservative than those that are media and/or pathway-specific. The primary screening methods that have been developed by the USEPA include PRGs, RBCs, and SSLs. These methods are described in more detail below. Each USEPA regional office may support the use of one or more of these screening approaches. State regulatory agencies may require the use of specific screening methods for sites within their jurisdiction.



**Preliminary Remediation Goals (PRGs).** Preliminary Remediation Goals (PRGs) are described in Part B of the RAGS (USEPA, 1991a). PRGs are used at the scoping phase of the risk assessment process. The residential soil PRG given in RAGS is derived from an estimate of the potential ingestion of soil. For industrial/commercial land uses, a soil PRG is calculated based on soil ingestion, as well as inhalation of volatiles released from soil and/or inhalation of airborne particulate matter. USEPA Region IX supports the use of PRGs with the modification that skin contact and inhalation (of volatiles or particulates) are also included as components of both the residential and industrial soil PRGs (USEPA, 1996b, 1998). Region IX also has a separate pathway-specific PRG for inhalation of contaminants in ambient air. The PRG methodology requires the use of certain chemical-specific data, such as diffusivity coefficients, to calculate a volatilization factor for each chemical contaminant. A nonchemical-specific "particulate emission factor" is used for chemicals that are not volatile.

**Risk-Based Concentrations (RBCs).** USEPA Region III (USEPA, 1996a) supports the use of RBCs which are similar to PRGs. USEPA Region III calculates a soil ingestion RBC for noncarcinogens (for children only) and for carcinogens (age-adjusted for a 30-year exposure period), but does not include inhalation or dermal contact as additional exposure pathways for contaminated soil. However, Region III calculates a pathway-specific RBC (inhalation only) for ambient air, as well as an RBC based specifically on ingestion of edible fish.

**Soil Screening Levels (SSLs).** USEPA's Office of Solid Waste and Emergency Response has developed soil screening guidance which is used to derive risk-based, site-specific SSLs (USEPA, 1996c). SSLs are concentrations of contaminants in soil that would be protective for residential exposure scenarios. For contamination of surface soils, SSLs are derived for two pathways, ingestion of soil and inhalation of fugitive dusts. For subsurface soils, SSLs are also derived for two pathways, inhalation of volatiles released from the soil and ingestion of ground water contaminated as a result of the migration of chemicals through the soil to the underlying aquifer.

### 1.2.3 Physical/Chemical Properties and Environmental Fate of Chemical Warfare Agents

Basic chemical and physical data for agents HD, Lewisite, GA, GB, GD, and VX are given in Table 1-1. The agents discussed in this report occur as liquids at ambient temperatures; however, HD freezes at approximately 57°F and, therefore, may not behave as a liquid in temperate climates. In terms of their absolute vapor pressures, all the agents except VX are considered to be volatile; that is, transfer from a liquid to a vapor state will occur. However, in terms of their potential for volatilization from an environmental matrix (i.e., subsurface soil or water), only HD is considered to be volatile by USEPA's definition of volatility (see Section 1.3.6).

HD is reported to be slightly soluble in water, but once dissolved is subject to rapid hydrolysis. According to Small (1984) the half-life for HD is less than 16 minutes and "does not vary appreciably in the typical environmental pH range"; however, MacNaughton and Brewer (1994) state that reversible reactions take place in acidic solutions and decomposition is accelerated in neutral and basic medium. For HD in equilibrium with water, the maximum rate of hydrolysis has been reported to be 104 mg/min/L at 25°C (Forsman et al, 1979). However, the reported rate of dissolution is only  $6.77 \times 10^{-8}$  g/cm<sup>2</sup>/sec (Rosenblatt et al., 1975). Thus, it was reported that the half-life of a 5 µL drop of HD in stirred distilled water at 20°C

would be 250 min (Sage and Howard, 1989), and a droplet of HD 1 cm in diameter would take 15 days at 18°C to decrease by one-half (Small 1984).

The hydrolysis of Lewisite is very rapid (Rosenblatt et al., 1975). In aqueous media, Lewisite exists primarily as 2-chlorovinyl arsonous acid (CVAA) (Major, 1998). Chlorovinyl arsenous oxide (Lewisite oxide) occurs as a dehydration reaction product of CVAA. Lewisite oxide is about 1% soluble in water (Rosenblatt et al., 1975). Though there are somewhat limited toxicological data on the breakdown products, Lewisite oxide it has been suggested that the toxicological data associated with Lewisite may be more representative of its degradation products (due to the extremely rapid hydrolysis).

The nerve agents are water soluble to varying degrees, with agent GB being miscible and the other nerve agents having solubilities ranging from 10 to 100 g/L. When dissolved in water, all the agents are subject to hydrolysis. Hydrolysis rates of the nerve agents are pH- and temperature-dependent (MacNaughton and Brewer, 1994). Data reviewed by MacNaughton and Brewer (1994) indicate that the hydrolysis of GB is slowest at pH 6-7 but much faster at higher or lower pHs. For GD, hydrolysis rates are similar over a pH range of 5-8. Because hydrolysis products may alter the pH of the solution, half-lives measured under pH-controlled laboratory conditions may not correspond to those occurring under ambient conditions. Although a half-life of >1000 hours has been reported for VX at pH 7, spontaneous half-lives of 80 and 57 hours have also been reported.

When applied to the surface of soils, the agents are generally nonpersistent. Persistence times for agents on soil are generally less than several weeks, but may be longer at low temperatures. Longer persistence times are likely when agents are buried in dry soil. Rosenblatt et al. (1995) estimated that even under the worst plausible conditions in a relatively dry but not totally water-free soil, agent GB would not be detectable after a month or less. Under similar conditions, the less volatile VX would not be detectable after about 3 months. When sprayed on soil, HD persists for several weeks (DA, 1974; Small, 1984); however, when buried in soil it may remain vesicant for several years or more (Small, 1984; Rosenblatt et al., 1995). HD buried in soil can become encapsulated in a polymeric coating formed with its hydrolysis products (Rosenblatt et al., 1995). These "capsules" are stable and nonmobile and prevent the enclosed mustard agent from undergoing further degradation. Additional information on the environmental fate of chemical warfare agents can be found in DA (1974), Small (1984), Sage and Howard (1989), MacNaughton and Brewer (1994), and Rosenblatt et al. (1995).

In summary, there are limitations with the data available to establish quantitative estimates of environmental parameters. That said, environmental fate and transport assumptions for a variety of industrial chemicals are also constrained by limited data and variability due to climate, moisture, pH, and other environmental conditions. Therefore, the fate and transport, including degradation, of chemicals in the environment is not accommodated in the existing risk assessment models described in this document. As the basic assumption of the chronic risk assessment model is that exposure to a chemical will occur over many years, potential chemical degradation in the short term may be a factor to consider when performing further analyses or assessment of the overall risk. This is especially true for the chemical agents described in this document, as they are generally not persistent. The information in Table 1-1 and the associated uncertainties with the risk model (i.e. consistent concentrations over the long-term) should therefore be incorporated into the risk management decision-making process.

Table 1-1. Physical/chemical/environmental properties of chemical warfare agents						
Property	HD	L	GA	GB	GD	VX
Primary exposure pathway	vapor/ contact	vapor/ contact	vapor/ contact	vapor	vapor	contact
Physical state	liquid	liquid	liquid	liquid	liquid	liquid
Molecular weight	159.08	207.32	162.1	140.1	182.2	267.4
Boiling point (°C)	217	190	245	158	198	298
Vapor pres. (mm Hg at 25°C)	0.11 0.165 <sup>g</sup>	0.58 <sup>g</sup> 0.40 (trans) 1.56 (cis)	0.07	2.94 <sup>g</sup>	0.40	0.0007
Water solubility (g/L)	0.920 0.8 <sup>g</sup>	0.5 <sup>e</sup>	98 50-100 <sup>g</sup>	miscible <sup>g</sup>	21 20-30 <sup>g</sup>	30 10-50 <sup>g</sup>
Liquid density (g/mL at 25°C)	1.27	1.88	1.08	1.09	1.02	1.0083
log Octanol-water partition coefficient (K <sub>ow</sub> )	1.37 <sup>a</sup>	NA <sup>c</sup>	1.18 <sup>b</sup>	0.15 <sup>b</sup>	1.02 <sup>b</sup>	2.09 <sup>a</sup>
Hydrolysis half-life (hr)	0.08 (acidic) 0.065-0.26 <sup>a</sup>	NA <sup>c</sup>	2 (pH 9) <sup>g</sup> 8.5 (pH 7) 2.5 (pH 7) <sup>g</sup> 7 (pH 5) 2.5 (pH 5) <sup>g</sup>	5 (pH 9) 0.5 (pH 9) <sup>g</sup> 70 (pH 7) <sup>g</sup> 250 (pH 6.5) <sup>g</sup> 47 (pH 6) 0.5(pH 5) <sup>g</sup>	60 (pH 10) 0.9 (pH 9) <sup>g</sup> 45 (pH 6.65) 40 (pH 7) <sup>g</sup> 40 (pH 5) <sup>g</sup>	~50 (pH 9) <sup>g</sup> 57 <sup>d</sup> 80 <sup>h</sup> 1000 (pH 7) <sup>g</sup> 2000 (pH 5) <sup>g</sup>
Persistence in soil	several wk <sup>a</sup> 1 yr+ <sup>f</sup>	ND	1 to 1.5 days	2.5 hr to 5 days < 1 month <sup>f</sup>	ND	2 to 6 days < 3 months <sup>f</sup>

SOURCES: DA, 1974, unless otherwise noted: for most values data points are for 20-25°C

<sup>a</sup> Values from Small (1984); hydrolysis half-lives at 20-25°C; soil persistence for agent applied to soil surface

<sup>b</sup> Estimated value from Britton and Grant (1988)

<sup>c</sup> Not available, cannot be calculated due to rapid hydrolysis

<sup>d</sup> Value from Szafraniec et al. (1990); unbuffered water, when dissolved VX causes an initial increase in the pH to 9

<sup>e</sup> According to Rosenblatt et al. (1975), solubility data for Lewisite are meaningless because of very rapid hydrolysis, which is limited by slow rate of dissolution

<sup>f</sup> Value from Rosenblatt et al. (1995); for worst plausible conditions

<sup>g</sup> Value from MacNaughton and Brewer (1994); hydrolysis of HD limited by rates of dissolution

<sup>h</sup> Value from Yang et al. (1990); spontaneous hydrolysis

### 1.2.4 Toxicity Values

For many environmental contaminants, USEPA has derived official oral RfDs, inhalation RfCs, and oral and inhalation slope factors which are made available to risk assessors through USEPA's IRIS or HEAST (USEPA, 1997c). This has not been the case for military-unique chemicals which may also occur as environmental contaminants. However, various exposure limits for the chemical agents (see Table 1-2) have been developed by the Army (e.g. general population air values and, recently, oral RfDs) which now permit the application of chronic risk assessment models to assessing chemical agent contamination.

<b>Table 1-2. Available reference doses, slope factors and inhalation exposure limits for chemical warfare agents</b>					
<b>Chemical</b>	<b>Oral RfD<sup>a</sup> (mg/kg/d)</b>	<b>Oral Slope Factor (mg/kg/day)<sup>-1</sup></b>	<b>Inhalation Slope Factor (mg/kg/day)<sup>-1</sup></b>	<b>General Public Air Exposure Limit<sup>d</sup> (mg/m<sup>3</sup>)</b>	<b>Inhalation RfD<sup>e</sup> (mg/kg/day)</b>
HD	$7 \times 10^{-6}$	$7.7^b$	$300^c$	$1 \times 10^{-4}$	$3 \times 10^{-5}$
Lewisite <sup>g</sup>	$1 \times 10^{-4}$	-	-	$3 \times 10^{-3}$	$8.6 \times 10^{-4}$
GA	$4 \times 10^{-5}$	-	-	$3 \times 10^{-6}$	$9 \times 10^{-7}$
GB	$2 \times 10^{-5}$	-	-	$3 \times 10^{-6}$	$9 \times 10^{-7}$
GD	$4 \times 10^{-6}$	-	-	$1 \times 10^{-6}^f$	$3 \times 10^{-7}$
VX	$6 \times 10^{-7}$	-	-	$3 \times 10^{-7}^h$	$9 \times 10^{-8}$

<sup>a</sup> Source: DA, 1996a

<sup>b</sup> Geometric mean of estimated slope factors; see Section 1.2.4 of this report for derivation

<sup>c</sup> DA (1996a); derived from an inhalation unit risk of  $8.5 \times 10^{-2}$  per  $\mu\text{g}/\text{m}^3$  (see USEPA, 1991b)

<sup>d</sup> DHHS (1988); DA (1990, 1991)

<sup>e</sup> Estimated from the air exposure limits using an inhalation rate of  $20 \text{ m}^3/\text{day}$  and a body weight of 70 kg

<sup>f</sup> Value estimated by Mioduszewski et al. (1998)

<sup>g</sup> The RfD for Lewisite was considered to be nonverifiable by the Strategic Environmental Research and Development Program (SERDP) Working Group; however, this value was approved as an interim value by the Office of The Surgeon General (OTSG), pending review by the Committee on Toxicology (COT).

<sup>h</sup> The CDC-based and current Army general population air limit is  $3 \times 10^{-6}$ ; recent technical evaluations suggest a potential future modification. Therefore, the potentially new value of  $3 \times 10^{-7}$  is used here. (USACHPPM, 1998)

The Centers for Disease Control and Prevention (CDC) have evaluated occupational and general public inhalation exposure limits for the nerve agents GA, GB, VX; the mustard agents H, HD, and HT; and Lewisite (DHHS, 1988). The Army has adopted these inhalation exposure standards (DA, 1990, 1991). Recent technical evaluations have verified the validity of the G-agent air standards but have suggested that the VX general population limit should potentially be lowered by a factor of 10 (USACHPPM, 1998). In this report the lowered VX limit ( $3 \times 10^{-7}$ ) is used in place of the existing standard ( $3 \times 10^{-6}$ ) to ensure conservatism should standards be changed. This modification did not, however, significantly impact the resulting value of the screening levels. These air exposure limits are used in this report as surrogate RfCs and are converted into inhalation RfDs (RfDi) using the standard exposure parameters of  $20 \text{ m}^3/\text{day}$  as an adult inhalation rate and 70 kg as an adult body weight. Toxicity values derived for adults are routinely used by

USEPA to develop screening values for scenarios where children are the primary receptors (i.e., soil ingestion) by including adjustments in the models, and this same approach is used in this report for the chemical warfare agents.

Under the sponsorship of the Army Environmental Center at Aberdeen Proving Ground, oral RfDs were derived for HD, Lewisite, GA, GB, GD, and VX (Opresko et al., 1998; see Table 1-2). These toxicity values have undergone extensive internal and external review, including that by the multi-agency Environmental Risk Assessment Program (ERAP) of the SERDP. The agencies participating in SERDP include the U.S. Army, U.S. Navy, U.S. Air Force, U.S. Department of Energy, and the USEPA. Following approval by ERAP, the oral RfDs were submitted to the U.S. Army OTSG, and were approved as interim values by that office on June 4, 1996 (DA, 1996a). They were similarly concurred with by the CDC (DHHS, 1997). As of March 1999, these toxicity values are undergoing review by the Subcommittee on Chronic Reference Doses for Selected Chemical Warfare Agents, COT, National Research Council. The final recommendations of the COT subcommittee should be available before the end of FY 99. The RfDs used in this report, therefore, may be subject to change following the completion of the COT review.

Agent HD is considered to be a human carcinogen (IARC, 1987; NTP, 1997). In evaluating the potential carcinogenic risks associated with HD incineration, the USEPA derived an inhalation unit risk for HD using chronic animal vapor exposure data as well as a relative potency approach based on short-term carcinogenicity studies (USEPA 1991b). No long-term animal carcinogenicity studies have been conducted from which a quantitative estimate of HD potency following oral exposures can be obtained (i.e., there is no experimentally derived oral slope factor). The relative potency value calculated by USEPA (1991b) can be converted to an oral slope factor of 95 (mg/kg/day)<sup>-1</sup>. This value was proposed as an interim slope factor for HD by OTSG (DA, 1996a). There are, however, other estimates of the HD slope factor. The relative potency Rapid Screening of Hazard (RASH) approach, as developed by Watson et al. (1989) can be used to derive an oral slope factor of 9.5 (mg/kg/day)<sup>-1</sup> using the current USEPA slope factor of 7.3 for benzo(a)pyrene (BaP). The RASH method has been validated as an acceptable method for estimating carcinogenic potency (Omenn et al., 1995). The carcinogenicity of HD has also been evaluated by Gaylor (1998) using several different methods (see Appendix B). In one approach, the slope factor was estimated from the relative potency value of Watson et al. (1989) and a new slope factor for BaP derived from a study by Culp et al. (1998). The resulting HD slope factor is 1.6 (mg/kg/day)<sup>-1</sup>. If the Culp et al. (1998) slope factor for BaP is applied to USEPA's highest relative potency value for HD, the resulting slope factor is 15.6 (mg/kg/day)<sup>-1</sup>. Gaylor (1998) also estimated HD slope factors of 5.0 and 2.6 (mg/kg/day)<sup>-1</sup> using linear extrapolations from benchmark doses producing forestomach hyperplasia in rats (Sasser et al., 1989a, 1989b), and a slope factor of 5.3 (mg/kg/day)<sup>-1</sup> using a method based on the maximum tolerated dose (Gaylor and Gold, 1995).

The different approaches described above yield HD slope factors of 1.6, 5.0, 2.6, 5.3, 15.6, 9.5, and 95 (mg/kg/day)<sup>-1</sup>, respectively. The Shapiro-Wilk test for normality was used to evaluate the distribution of these values. The resulting normality value was 0.58007 ( $p = 0.002$ ), indicating that these values are not distributed normally. Log transformation of the values yielded a normality value of 0.933577 and a  $p$  value of 0.601, indicating that the values are distributed log normally. Therefore, the geometric mean of 7.7 (mg/kg/day)<sup>-1</sup> is considered to be the best overall measure of the slope factor for HD. It should be noted, however, that the slope factor of 95 (mg/kg/day)<sup>-1</sup> could be considered an outlier in the available data set (D. Gaylor, FDA, personal communication to A. Watson, ORNL, 9 June, 1998). If this value is not used in the

calculation, the final geometric mean based on the remaining six values would be  $5.0 \text{ (mg/kg/day)}^{-1}$ . In the HBESL calculations in this report the more conservative value of  $7.7 \text{ (mg/kg/day)}^{-1}$  is used.

Issues surrounding the carcinogenicity of HD and the derivation of slope factors are currently being evaluated by the COT Subcommittee on Chronic Reference Doses for Selected Chemical Warfare Agents.

Although an oral RfD was derived for Lewisite ( $1 \times 10^{-4} \text{ mg/kg/day}$ ) (Opresko et al, 1998), it was the conclusion of the Strategic Environmental Research and Development Program (SERDP) Working Group that this RfD was not verifiable because of deficiencies in the available toxicity data. The Working Group recommended that the RfD for inorganic arsenic ( $3 \times 10^{-4} \text{ mg/kg/day}$ ) should be used instead. Because these values are so similar and the fact that the Lewisite RfD was recommended by the Army Office of the Surgeon General (DA 1996a) for use as an interim value, the derivation of  $1 \times 10^{-4} \text{ mg/kg/day}$  is used in this report, pending the final recommendations of the COT.

There are no epidemiological or experimental data indicating that Lewisite is carcinogenic in humans or animals; however, the Lewisite breakdown product, inorganic arsenic, is considered to be carcinogenic. Slope factors and cancer-based screening values (PRGs and SSLs) are available for inorganic arsenic (USEPA, 1998). Specific calculations for the Lewisite screening values were done using the interim RfD (noncancer). Sites where Lewisite is a potential concern should include evaluation for inorganic arsenic to include the carcinogenic effects associated with this compound.

Dermal chronic toxicity RfDs are not currently available for chemical agents, as is the case with the majority of industrial/agricultural compounds. Using the EPA Region IX method (which assesses the dermal contact pathway), oral based RfDs are converted to (or used as surrogates for ) dermal RfDs where no other information is available (USEPA1996b). In this report, available data on acute dermal effects of the agents were used to modify dermal RfDs as appropriate. For example, because the standard EPA Region IX method results in a dermal Lewisite RfD of  $7 \mu\text{g}$ , which is above a potential acute dermal effect level, the Lewisite screening values in this report were calculated using a dermal RfD derived from existing acute dermal toxicity data, resulting in a more conservative estimate. This was accomplished by adjusting the reported effect level of  $3.5 \mu\text{g}$  (see Section 1.3.8) by a standard factor of 10 to arrive at an estimated no-effect level of  $0.35 \mu\text{g}$ . Because dose-response data are not available to be certain that  $0.35 \mu\text{g}$  is a no-effect level, an additional Modifying Factor of 3 was applied, resulting in a value of  $0.12 \mu\text{g}$ . For a 70 kg person this is equivalent to a dermal RfD ( $\text{RfD}_d$ ) of  $0.0017 \mu\text{g/kg}$  body weight ( $0.0000017 \text{ mg/kg}$ ).

### 1.3 LIMITATIONS

The HBESLs calculated in this report are to be used to *screen* sites with potential health risks. Though they are considered conservative, the actual degree of conservatism will vary depending on the unique site situation to which an HBESL is being applied. A proper balance in the conservatism of assumptions and uncertainties is necessary to ensure that decision-making is conservatively safe, but not excessively so. The major potential flaws/uncertainties in the assumptions underlying the various HBESLs described in this document are discussed along with presentation of the different models and the calculated HBESLs values. In general, these “flaws” depict a fundamental problem with using standardized algorithms and assumptions - that unique site and chemical characteristics will be overlooked. In this way, excessive over-conservatism can lead to potential unnecessary scrutiny, concern, or even remedial action at a given site. On the other hand, underconservative assumptions could potentially cause decision-makers to over-look a potential health concern. But despite this limitation, the use of HBESLs, as indicated by the referenced approaches used in this document, is the currently accepted approach in the environmental assessment and remediation field and serves a useful purpose in focusing environmental health decision-making. *For the best decision-making, however, the underlying assumptions and associated limitations must be understood before applying the HBESLs in the decision-making process.*

When an HBESL is exceeded, additional analyses should be undertaken with more site-specific data, which in most cases leads to a complete baseline risk assessment. However, before the HBESLs are even applied to make such decisions, certain criteria must first be met. An initial site evaluation is necessary to ensure that the assumptions used to derive the HBESLs are at least as, if not more, conservative than what reasonably can be expected from the site in question. Evaluation is necessary to ensure that no potential exposure pathways have been overlooked and that no unique population, chemical, or environmental factors exist that require more site-specific HBESLs. Other components of the model need to be verified for site-specific application to ensure that the designated level of risk is “acceptable” to site stakeholders; to ensure that acute concentrations are not of concern at the site; and to verify that ground-water contamination is not a realistic possibility. Furthermore, because the HBESLs are based solely on human health endpoints, additional evaluation may be necessary in order to make determinations about potential ecological effects. A more detailed discussion of these issues and other somewhat “flawed” aspects of the risk assessment models, assumptions, and screening approaches are discussed in Sections 1.3.1 through 1.3.10.

#### 1.3.1 Exposure Scenarios

Although the HBESLs developed in this report represent a first step in the risk assessment process, they also provide a certain level of site specificity in terms of the potential exposure scenarios evaluated. As stated, two scenarios are generally addressed by USEPA: 1)residential and 2)industrial scenarios. Residential exposure scenarios are established because these result in particularly conservative values which are protective for most all other exposure situations. However, as many sites are realistically not used or going to be used as residential property, the USEPA also provides screening values for industrial/commercial scenarios. While considered less conservative than the residential-based screening values, the industrial-based values still offer conservative protection for the given scenario. A determination can be made from general site information regarding the appropriate selection of the type (industrial or residential based) of screening values to be used in the screening assessment process.

The calculation of chemical warfare agent HBESLs for both residential and industrial scenarios are demonstrated in the main body of this document. However, the Army may need to perform site specific risk assessments to determine “safe” levels of contaminants for other types of scenarios. The higher degree of variation in site-specific parameters for such scenarios makes it difficult to establish representative, yet conservative, ‘screening levels’. Examples of such scenarios include: (1) trespassers (Appendix C), and (2) evaluation of potentially contaminated land being used for agricultural/grazing purposes (Appendix D). While establishment of specific screening level values for such scenarios is precluded given current data limitations, the identified appendices present discussions of the various considerations and limitations of applying the described risk assessment models to such unique situations.

Additional scenarios that are not included in this report are those involving site-specific military uses (e.g., training operations), or military or nonmilitary recreational uses (e.g., parkland, hunting and/or fishing areas). HBESLs for such scenarios may be developed in the future as the need arises. In the interim, preliminary risk assessments may be generated for these scenarios by modifying various parameters established in this document. For example, to establish the degree of acceptable contamination at military training sites, the HBESL for an industrial scenario may be “borrowed” and certain modifications made to better reflect the uniqueness of the scenario. These modifications may be necessary because of an assumption that soldiers spend more time in contact with soil than typical industrial workers due to time spent in close contact with the soil and mud during training exercises and maneuvers, and may therefore have increased skin contact, ingestion, and/or inhalation exposures. On the other hand, soldiers may not be expected to spend every workday in the field, so their exposure duration and frequency may need to be modified to reflect a more realistic scenario.

Certain scenarios described in this document (such as trespasser) demonstrate that the chronic risk assessment model may fail to accommodate the “acute” risk from a single “hot spot” of concentrated chemical agent. In situations where the calculated HBESL is at levels which approach potential acute toxicity concerns, it may be more prudent to consider the assessment of individual hot spots to ensure that the potential of acute risk is mitigated at these higher concentration levels. Only in situations where the agent is reasonably assumed to be homogeneously adsorbed or otherwise mixed in with the matrix (e.g., possibly waste soil or even more homogenous as in liquid matrices) is the use of the risk assessment model appropriate.

### 1.3.2 Target Cancer Risk Levels

An HBESL derived for the only carcinogenic agent assessed, HD, was determined not only by the exposure assumptions used and by the chemical-specific CSF [which reflects the “potency” of the chemical to cause cancer (see Section 1.2.4)], but also by the target cancer risk level (TR). The TR value in the risk assessment model reflects the increased lifetime chance of developing cancer due to exposure to the chemical of concern. In establishing screening levels, the TR represents an “acceptable” increase in the number of cancer cases in a given population. In establishing the HBESLs in this report, TRs of  $10^{-5}$  for residential



populations and  $10^{-4}$  for industrial/commercial scenarios are used. The following paragraphs outline the justification for the values chosen.

The TRs chosen for the development of the HBESLs for HD fall within the  $10^{-4}$  and  $10^{-6}$  acceptable range as determined by USEPA (1991a). While the methods described in this document, namely the PRGs, SSLs, and RBCs, use a point of departure of  $10^{-6}$  for both the residential and commercial/industrial scenarios, this is not necessarily appropriate for most chemical warfare agent-impacted sites. The USEPA has not promulgated a single acceptable level of carcinogenic risk; however, it has indicated that "for known or suspected carcinogens, acceptable exposure levels are generally concentration levels that represent an excess upper bound lifetime cancer risk to an individual of between  $10^{-4}$  and  $10^{-6}$ ." Furthermore, there is evidence that Federal agencies have tended to use the middle and upper part of this risk range for regulatory decisions affecting the general population. In reviewing public health policy decisions, Anderson et al. (1983) found that most regulatory decisions reduced risks to near  $10^{-5}$ . In decisions concerning hazardous waste sites where the affected geographic area is small and where population risks are presumably also small, Travis et al. (1987) found that past regulatory actions indicated that  $10^{-4}$  was the *de minimis* risk level for these sites, with *de minimis* risk being an acceptable level that is below regulatory concern.

For residential scenarios, some states require the use of a  $10^{-6}$  target risk goal; however, others have adopted higher acceptable risk levels for environmental standards for the general public. In California, under Proposition 65 (the Safe Drinking Water and Toxic Enforcement Act), lifetime cancer risks less than  $10^{-5}$  are not considered significant (Pease et al., 1990). Under the Ohio Voluntary Action Program, an acceptable risk level of  $10^{-5}$  was adopted for both single and multiple chemical exposures for residential and commercial/industrial land use (Lohner, 1997). The State of Minnesota uses a  $10^{-5}$  lifetime cancer risk in deriving health-based limits for protection of ground water (Minnesota Rules Chapter 4717.7300). The State of Tennessee uses a  $10^{-5}$  risk level for surface water quality criteria (Tennessee Water Quality Standards, Chapter 1200-4-3-.03). Similarly, Texas (Water Quality Standards, Section 307.6) and Virginia (9 Virginia Code 25-260-140) use  $10^{-5}$  for surface water quality standards. For regulating inhalation exposures, the State of Maryland has codified  $10^{-5}$  as an acceptable risk level for exposures to the chemical warfare agent HD [Title 26.11.15, Part .01 A(8)].

A TR of  $10^{-5}$  was chosen for residential scenarios not only because it falls within the USEPA range of acceptable risk levels and is an established acceptable risk level by many states, but also for the following reasons:

- Chemical warfare agent-impacted sites are expected to be affected by a single compound, namely the agent. The screening methods used to develop the HBESLs are typically used at sites that are impacted by numerous substances.
- HD is relatively immobile in the environment.
- Exposure to chemical agent is expected to be quite limited because most chemical-agent impacted sites have restricted access.

- Analytical detection capabilities at concentrations driven by a  $10^{-6}$  TR are questionable. Ultimately the benefits of choosing a lower TR will be lost, because the HBESL based on a TR of  $10^{-6}$  may be lower than the detection limit for HD in an environmental medium. *It is a common problem, even when evaluating samples for industrial chemical contaminants, that analytical detection capabilities will exceed the intended health-based goal particularly in soil or 'dirty' matrices.*

A TR of  $10^{-4}$  was chosen for industrial scenarios for the same reasons outlined above. Additionally, although a risk level of  $10^{-6}$  is the standard default used by USEPA for deriving PRGs for industrial/commercial land use scenarios (USEPA, 1991a), occupational exposure standards have been historically set at levels corresponding to much higher risk levels. The Occupational Safety and Health Administration (OSHA) establishes exposure limits at the "lowest feasible level which is reasonably necessary or appropriate to eliminate significant risk." In general, OSHA considers  $10^{-3}$  a threshold of significant risk (Rodricks et al., 1987; Graham, 1993), and the agency usually does not regulate lower risks because of feasibility limitations (Lohner, 1997).

In the case of benzene, the OSHA 8-hour time-weighted average (TWA) standard is 1 ppm (Title 29, Code of Federal Regulations, Part 1910). This exposure is equivalent to  $3.24 \text{ mg/m}^3$ , or  $771 \text{ } \mu\text{g/m}^3$  when converted into a 24 hours/day, 7 days/week exposure. The inhalation unit risk for benzene is  $8.3 \times 10^{-6} (\text{ } \mu\text{g/m}^3)^{-1}$  (value from IRIS, USEPA, 1997a). Therefore, the cancer risk at the current OSHA standard is  $6.4 \times 10^{-3}$  [using the standard equation, Risk = Dose x Unit Risk; i.e.,  $771 \text{ } \mu\text{g/m}^3 \times 8.3 \times 10^{-6} (\text{ } \mu\text{g/m}^3)^{-1}$ ]. The current OSHA standards for vinyl chloride and inorganic arsenic are 1 ppm ( $2.60 \text{ mg/m}^3$ ) and  $10 \text{ } \mu\text{g/m}^3$ , respectively; the inhalation unit risks are  $8.4 \times 10^{-5}$  and  $4.3 \times 10^{-3}$  (from IRIS or HEAST), and the resulting cancer risk levels are  $5.2 \times 10^{-2}$  and  $1.02 \times 10^{-2}$ .

Significant risk in occupational exposures must be viewed in the context of the number of individuals who may be exposed. Establishing a standard based on a one-in-one million risk when only a small number of individuals may be exposed may not be a realistic risk management decision. Furthermore, long-term exposures to HD-contaminated soil or water are unlikely at commercial/industrial sites.

Due to the reasons discussed above, TRs of  $10^{-5}$  for residential populations and  $10^{-4}$  for industrial/commercial scenarios were used to calculate the HBESLs. The determination of TRs for the development of screening levels requires that a single conservative value be selected for each scenario (i.e., industrial/commercial or residential). The TRs selected for development of the HD HBESLs fall within the range generally accepted as "conservative."

When using the HBESLs developed in this document, it should be noted that an acceptable risk is not a scientifically derived value. Rather, it is a judgment decision properly made by those exposed to the hazard or their designated health officials (Kelly, 1991). Therefore, while this document has used a predetermined level of "acceptable risk," application of the carcinogenic HBESL must incur stakeholder involvement to determine whether a lower or higher level of risk is a more appropriate decision pending site-specific circumstances.

### 1.3.3 Potential for Chemical Agent Migration to Ground Water

The HBESL that evaluates the potential for contamination of ground water as a result of migration of a chemical through soil (OSWER-derived SSL) requires the use of a set of simplifying assumptions which may not be applicable if a chemical's distribution in soil is very localized, if it is strongly bound to soil organics or inorganics, or if its residence time in soil is relatively short (i.e., if it is subject to rapid degradation through abiotic or biological processes). In such cases the development of a generic soil SSL based on the potential for migration to ground water may not be appropriate, and site-specific HBESLs should be considered. Of the agents evaluated in this report, the nerve agents are not expected to be persistent in soils. Studies reviewed by Small (1984) indicate that 90 percent of GB applied to soil will be lost in 5 days, and a similar decrease in VX will occur in 15 days. Soil persistence time periods under worst plausible conditions were estimated to be 1 month or less for GB and 3 months or less for VX (Rosenblatt et al., 1995). Of the nerve agent degradation/breakdown products, only EA-2192 is considered to be both environmentally persistent and sufficiently toxic to be a significant ground-water contaminant (see Appendix F).

The potential for HD to contaminate ground water is extremely low because the agent, when dissolved in water, is subject to rapid hydrolysis (see Table 1-1). Furthermore, although HD may remain in soils for long periods of time, it is known to form relatively nonmobile polymeric aggregates with its hydrolysis products; therefore, migration downward through the soil to ground water is unlikely. HD has not been found in any ground-water monitoring samples; however, its more stable but much less toxic hydrolysis product, thiodiglycol, has been found in ground water.

Lewisite dissolved in water hydrolyzes almost immediately to the soluble but nonvolatile 2-chlorovinyl arsonous acid (CVAA). Lewisite oxide may then result as a product of a dehydration reaction. Lewisite itself is not expected to be found in ground water (nor is Lewisite oxide); however, evaluation of potential ground-water contamination should consider the more soluble CVAA or secondary degradation products such as inorganic arsenic (see Appendix F).

Because rates of degradation are not incorporated into USEPA's methodology for deriving SSLs for migration to ground water, these screening levels do not provide an accurate estimate of the risk of ground-water contamination by reactive contaminants. The potential for chemical agent migration to, and movement through, ground water was assessed using two mathematical models, VLEACH and a horizontal flow model incorporating chemical-specific rates of hydrolysis. A description of the models and the results are presented in Appendix E. The models indicate that, in general, ground-water contamination by the agents is very unlikely except under extreme circumstances (i.e., shallow aquifer and high ground-water flow). However, even for those scenarios where the agents could theoretically reach the aquifer, horizontal transport through the ground water is predicted to be only a few hundred meters or less before the agent concentrations are reduced to levels that are below acceptable drinking water HBESLs.

### 1.3.4 Potential for Chemical Agent Contamination of Drinking Water

As noted in the previous section, the likelihood of agents reaching ground water is very small and, consequently, the potential for contamination of drinking water derived from a ground-water source is even more remote. Agents present in surface waters as a result of runoff from contaminated soils would also be subject to hydrolysis and degradation. Hydrolysis half-lives of the nerve agents are less than 80 hours at environmental pH values. Furthermore, hydrolysis of some agents, such as GB and GD, is likely to be enhanced during standard water treatment procedures, since it has been shown experimentally that hypochlorite catalyzes the reaction (see Rosenblatt et al., 1995, for review). Drinking water contamination by stable agent degradation products may be a more appropriate consideration.

When dissolved in water, the half-life of agent HD is less than 15 minutes due to its rapid hydrolysis to thiodiglycol (see Section 1.2.3). Thiodiglycol is relatively stable in water and might be used as a marker for previous water contamination with HD. HD may, however, be persistent in surface waters if present in large amounts. This is due in part to the slow rate of dissolution of HD as well as to the possible encapsulation of HD by stable oligomeric hydrolysis products which prevent further dissolution and hydrolysis (MacNaughton and Brewer, 1994; Rosenblatt et al., 1995). HD is denser than water; therefore, undissolved agent is likely to settle to the bottom of water bodies where, if undisturbed and encapsulated, it may remain for an extended period of time.

As stated previously, Lewisite hydrolyzes rapidly to CVAA. Information was not available on the persistence of CVAA. Since Lewisite oxide is a product of dehydration reaction, it would also not be expected to be present in water. Given the rapid hydrolysis of Lewisite, it has been suggested that its toxicity may in part be attributed to these breakdown products.

### 1.3.5 Breakdown Products of Environmental Concern

Environmental fate and transport processes will, to a great degree, determine the relevance of particular HBESLs for specific chemical compounds. In general, the greater the reactivity of a chemical, the less likely that it will remain for very long in the environment in an unchanged state. Soil HBESLs should be evaluated in terms of the expected soil persistence of the contaminants (see Table 1-1). For very volatile or reactive contaminants, the residence time in the soils may be so short that the potential for chronic exposures will be very low. In such cases, and particularly at sites where the contaminants have weathered over a long period of time, the presence of stable degradation products may be more relevant for health risk assessments. Several of the degradation products of the chemical agents discussed in this report are evaluated in Appendix F. The information in Appendix F is not all inclusive of the degradation products that may be found in the environment, but describes compounds that may be relatively persistent and/or believed to be significantly toxic and which may, therefore, need to be investigated at a particular site. Extensive lists of agent breakdown and degradation products under several different conditions (e.g., hydrolysis, decontamination processes, combustion, and microbial degradation), including information on toxicity and availability of toxicity values (RfDs and slope factors), are provided in DA (1988), and Munro et al. (Submitted for publication, Dec 1998). These lists should be reviewed for site-specific applicability; however, it should be emphasized that a site investigation should not involve excessive sampling and analysis for all possible degradation products since the identification of trace amounts of nontoxic or nonpersistent chemicals would not provide any more useful information. Most degradation products of the chemical agents are less toxic

than the parent compounds. Therefore, a determination of key constituents of concern should be made initially to focus the risk assessment on critical areas and to avoid being hampered by unusable or unnecessary data.

### 1.3.6 Volatility of Chemical Agents in Water and Soil

The potential for a chemical to volatilize from water is not solely dependent on its vapor pressure. It is also a function of the chemical's water solubility and its tendency to partition between water and air. The USEPA determines whether volatilization from water is relevant for a specific chemical by using each chemical's Henry's Law Constant (H). Henry's Law Constant is the ratio of a chemical's volatility to its water solubility. According to USEPA, a contaminant with a Henry's Law Constant less than  $1 \times 10^{-5}$  atm-m<sup>3</sup>/mol and a molecular weight greater than 200 is not likely to pose an inhalation hazard as a result of volatilization from drinking water in a residential setting. Henry's Law Constants were estimated for the chemical warfare agents (see Appendix A and Table 2-3). Using these criteria, the only agent that is a potential inhalation hazard from drinking water is HD ( $H = 2.4 \times 10^{-5}$  atm-m<sup>3</sup>/mol and molecular weight = 159.08). However, several of the agents have higher vapor pressures than HD. GB, in terms of its absolute vapor pressure (2.9 mm Hg), is normally considered to be more volatile than HD (vapor pressure 0.11 mm Hg). Although it is counterintuitive to think that GB in water would not be a vapor hazard, chemicals with a similar vapor pressure have also been classified by USEPA as being "nonvolatile." For example, butanol has a vapor pressure of 6.7 mm Hg, but is considered by USEPA Region IX as being "nonvolatile" for the purposes of calculating drinking water PRGs (USEPA, 1998). This is because its water solubility is quite high (63,000 mg/L) resulting in a low Henry's Law Constant of  $8.81 \times 10^{-5}$  atm-m<sup>3</sup>/mol. Because agent GB is miscible with water, it also has a very low estimated Henry's Law Constant ( $5.34 \times 10^{-7}$  atm-m<sup>3</sup>/mol), and thus also fulfills USEPA's functional definition of being relatively nonvolatile from water. Although HD might be considered potentially volatile from water, its rapid rate of hydrolysis is likely to limit such losses (see Section 1.3.4).

The Henry's Law Constant of a chemical is also used by USEPA to determine if a contaminant is a potential inhalation hazard as a result of volatilization from subsurface soils (this approach is not appropriate for surface spills). Information in the Soil Screening Guidance document (USEPA, 1996d) indicates that this method is based on the assumption that, at relatively low concentrations, chemicals in subsurface soils will partition between soil-pore water and soil-pore air, depending on their water solubility and volatility. Thus, those chemicals with a low Henry's Law Constant (less than  $1 \times 10^{-5}$  atm-m<sup>3</sup>/mol) are more likely to remain in soil pore water. As noted above, however, this conclusion is counterintuitive for chemicals with high vapor pressures, and its applicability to every-day soils may be questionable. Thus, there is some degree of uncertainty surrounding the assumption whether or not a chemical with both a relatively high vapor pressure and a relatively high solubility, such as GB, would represent an inhalation hazard when buried in soil. According to USEPA methods, it would not.

Although HD has an estimated Henry's Law Constant slightly greater than  $1 \times 10^{-5}$  atm-m<sup>3</sup>/mol, volatilization from soils is likely to be limited by its rapid hydrolysis and by the formation on its outer surface of a polymeric coating (formed with its hydrolysis products) which prevents volatilization. At a site at Aberdeen Proving Ground, where the soil is known to be heavily contaminated with HD, an innovative biological monitoring technique has not revealed any evidence of atmospheric contamination (Rouhi, 1998).

### 1.3.7 Multiple Pathway Exposures

The HBESL that incorporates the greatest number of exposure pathways for a residential scenario (e.g., soil PRGs), is likely to result in the lowest screening values. The appropriateness of a multipathway HBESL is, however, dependent on several factors, including: 1) whether all exposure pathways are relevant for a given contaminant, 2) whether the same toxic endpoint occurs regardless of the exposure route, and 3) whether the appropriate toxicity values (RfD or slope factor) are available for each exposure route (or whether they can be reasonably estimated by means of route-to-route extrapolation). In situations where the target organ is different for each exposure route, it may be inappropriate to calculate a multipathway HBESL. For the systemically absorbed, cholinesterase-inhibiting nerve agents, multipathway evaluations are appropriate. In the case of the vesicants HD and Lewisite, the target organs for the various exposure pathways may not be identical if the agents are not absorbed systemically. In the case of low-level oral exposures, the toxic effect is on the lining of the gastrointestinal tract; following dermal exposures, it is on the skin; and for exposures to vapors, it is likely to be on the respiratory tract and/or the eyes and skin. The effects for each of these pathways would not be expected to be additive except possibly in the case of skin exposures by vapor or contaminated soil; but even in such situations, the same location on the skin would have to be affected. Multipathway HBESLs for HD or Lewisite are likely to result in conservative values.

### 1.3.8 Acute Toxicity Considerations

Care must be used in deriving HBESLs for chemical agents for relatively short-term exposures (e.g., trespasser scenario described in Appendix C of this document) to ensure that such HBESLs do not approach acutely toxic levels. The latter possibility exists because the HBESLs are derived from chronic RfDs; however, a linear dose-toxic response relationship may not exist when extrapolated to scenarios involving infrequent exposures, such as the trespasser HBESLs. The following is a summary of the available information on no-effect levels and on exposure levels associated with minimal acute toxicity. A comparison of minimum effect levels and calculated HBESLs for each chemical warfare agent is presented in Chapters 4-9 and in Appendix C.

**Dermal Exposures.** Only one HBESL (soil PRG) quantitatively addresses the issue of dermal exposures. For chemical warfare agents that are nonvolatile and readily absorbed through the skin (e.g., VX) or those that are vesicants (HD and Lewisite), this pathway is likely to be of great concern. For VX, as little as 0.32 mg applied to the skin may cause a toxic response. Mild signs of toxicity occurred in 1 percent of the tested individuals when this amount of pure VX was applied to the forearm (DA, 1974). A dose of 5 µg/kg (0.35 mg for a person weighing 70 kg) applied to the cheeks or earlobes resulted in signs of toxicity in about half of the tested individuals (Sim, 1962). In tests where VX was applied to polyurethane-painted steel surfaces, residual amounts of 20-40 µg VX produced toxic signs in rabbits (body weights 2.06-3.85 kg) following direct skin contact for 60 minutes; residual levels of about 10-20 µg were not toxic (Manthei et al., 1985).

For HD, human data are available on minimum effects levels for percutaneous exposures. Based on data generated at the University of Chicago Toxicology Laboratory, Landahl (1945) reported a median threshold blistering dose of 32 µg for purified H and 38 µg for Levinstein H. The data were reevaluated by Reutter and Wade (1994) who reported an ED<sub>50</sub> of 33.7 µg with a slope of 2.01 for H and an ED<sub>50</sub> of 38 µg for Levinstein H. Landahl (1945) also reported on the frequency of erythema in the exposed subjects. At the

lowest test dose of 2.5 µg, 87 of 209 individuals exhibited erythema, and 5 of the 209 exhibited blistering. An ED<sub>50</sub> of 2.8 µg/cm<sup>2</sup> for erythema was estimated from these data (Reutter, 1998).

Several studies have evaluated the potential hazards associated with skin contact with surfaces contaminated with HD (Manthei et al., 1983, 1986, 1988). In tests using polyurethane-painted steel plates, residual amounts of HD estimated to be as low as 20 µg were shown to be capable of causing erythema, edema, and eschar formation when the plates were applied to the clipped skin of rabbits for 60 minutes (Manthei et al., 1983). The effective dose was estimated from the initial application of 0.5 mg adjusted for a maximum 96 percent (minimum 62.2 percent) loss of agent by volatilization in controls during a 30-minute aging period prior to testing. Similarly, in studies where concrete was contaminated with HD, a residual HD level of about 20 µg was shown to cause primary skin irritation in clipped rabbits following a 60-minute contact period (Manthei et al., 1986). In a later study, Manthei et al. (1988) concluded that as little as 10 µg of HD will cause observable skin irritation in clipped rabbits after 60 minutes of direct contact. Manthei et al. (1988) also found that the clipped skin of swine was less reactive to HD than rabbit skin. However, Henry (1991) reported that rabbits were 8-10 times less sensitive than humans, and, in a review of the available toxicity data, Reutter and Wade (1994) concurred with this conclusion. Thus, the overall human and animal data indicate that HD doses of only a few micrograms (e.g., an estimated 2 µg) are likely to cause erythema in a large percentage of exposed individuals, and this dose level may even cause vesication (blistering) in some sensitive individuals. It should be noted that the dose of a few micrograms must be received in a single discrete exposure.

For GB, Grob et al. (1953) applied a 0.3 mL aqueous solution containing 6 mg GB to the forearm of a 96-kg individual. The solution was allowed to evaporate. There were no signs or symptoms of toxicity and no changes in blood cholinesterase (ChE). Grob et al. (1953) also reported that 20 mg of agent dissolved in propylene glycol and applied for 3.5 hours under a cup to the forearm caused no signs or symptoms of toxicity but did result in a 22 percent reduction in red-blood cell-ChE activity (to 78 percent of the control value).

For GA and GD, information on minimum effect levels (MELs) for percutaneous exposures was not readily available<sup>2</sup>. MELs were estimated by extrapolation from percutaneous LD<sub>50</sub> values. For VX, the ratio of the MEL (0.32 mg) and the percutaneous LD<sub>50</sub> value (10 mg) is 0.032. This same ratio can be used to estimate MELs for GA and GD. It should be noted, however, that this approach is used only to derive a rough approximation of the MELs in the absence of more specific data. The ratio approach would be expected to provide accurate estimates of MELs for agents with similar dermal dose-response curves; however, such dose-response information was not available for evaluation. For GD, the estimated percutaneous LD<sub>50</sub> value for humans is 350 mg for bare skin (DA, 1974), and, based on the MEL/LD<sub>50</sub> ratio for VX, the estimated MEL for GD is 11 mg. For GA, the percutaneous LD<sub>50</sub> value for humans is 1000-1500 mg (DA, 1974), and, based on the same ratio, the estimated MEL is 32-48 mg. In comparison, Freeman et al. (1954) reported that a dose of about 5 mg GA/kg body weight (about 400 mg) applied to the

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<sup>2</sup>Reutter (1998) identified several references pertinent to the evaluation of the acute percutaneous toxicity of GB and GD; however, copies of these references were not provided to the authors of this report, and, because they were not readily available, could not be included in this analysis.

skin would result in inhibition of blood cholinesterase, but would not cause clinical signs of toxicity. Therefore, the MEL estimated from the LD<sub>50</sub> data appears to be a relatively conservative value.

Minimum effect levels for percutaneous exposures to liquid Lewisite were not found in the available literature. However, Landahl (1945) reported that the median threshold blistering dose in a human study was 14 µg. In addition, Landahl (1945) reported that 29 out of 93 individuals exhibited erythema at the lowest study dose of 3.5 µg. In this study, 8 of the 93 individuals exhibited blistering, suggesting that the minimum effects level may be only a few micrograms. Exposure to a vapor concentration of 200 mg/m<sup>3</sup> for 30 minutes causes skin lesions in humans and 1 mg/m<sup>3</sup> for 30 minutes causes eye lesions in rabbits (DA, 1974).

**Oral Exposures.** In tests on humans, single oral doses of 2-4.5 µg VX/kg produced gastrointestinal symptoms in 5 of 32 individuals (Sidell and Groff, 1974). No signs of toxicity were seen in 16 individuals receiving 1.43 µg VX/kg/day for 7 days (in four doses per day of 500 mL drinking water). Assuming a body weight of 70 kg, the total daily dose would be 100 µg in 2 L of water, or a concentration of 50 µg/L. A single oral dose of 0.022 mg GB/kg produced mild signs of toxicity in humans, and a dose as low as 0.002 mg/kg reportedly caused excessive dreaming and talking during sleep (Grob and Harvey, 1958). For a person weighing 70 kg, the latter dose equals 0.14 mg and would correspond to a drinking water concentration of 0.07 mg GB/L, assuming an ingestion rate of 2 L/day. MELs for oral exposures to GA and GD were estimated from their acute toxicity (see Appendix G) to be 2.65 and 0.63 times that of GB, respectively. The resulting MEL for GA is 0.37 mg, corresponding to 0.16 mg/L for tapwater; the resulting MEL for GD is 0.09 mg, corresponding to 0.045 mg/L.

No information is available on MELs for ingested HD in humans. In rats, a daily dose of 2.5 mg/kg (about 0.8 mg/animal) for 14 days resulted in severe damage to the gastric mucosa (Hackett et al., 1987). Rats dosed subchronically with 0.03 mg HD/kg/day (approximately 0.01 mg total dose for rats weighing 0.35 kg) exhibited no signs of toxicity in one study (Sasser et al., 1996) and only mild signs of toxicity following 13 weeks of exposure (Sasser et al., 1989a). Estimates of MELs for orally administered Lewisite in laboratory animals range from 0.07 to 2 mg/kg/day (reviewed in Opresko et al, 1998).

**Inhalation Exposures.** Using experimental human data from a study by Kimura et al. (1960), McNamara et al. (1973) estimated that an intravenous (i.v.) dose of 0.1 µg VX/kg would have no effect on RBC-ChE activity. For an individual weighing 70 kg and breathing 15 L/minute, this i.v. dose converts to a VX concentration x time (Ct) of 0.47 mg-min/m<sup>3</sup> (McNamara et al., 1973). In studies conducted by Bramwell et al. (1963) individuals were exposed to VX (head and neck only) to Cts of 0.6 to 6.4 mg-min/m<sup>3</sup>, without respiratory protection. At Cts of 0.6-1.7 mg-min/m<sup>3</sup> (0.2-0.57 mg/m<sup>3</sup> for 3 min), RBC-ChE was depressed 10-22 percent; at Cts of 4.8-6.4 mg-min/m<sup>3</sup> (0.8-1.06 mg/m<sup>3</sup> for 6-7 min), RBC-ChE was depressed 44-70 percent. Some of the exposed individuals exhibited miosis, even with their eyes closed. Rhinorrhea occurred in 14 of the 19 tests.



Baker and Sedgwick (1996) reported that in individuals exposed to 0.5 mg GB/m<sup>3</sup> for 30 minutes, small changes were seen in single-fiber electromyography, and some individuals exhibited miosis and mild dyspnoea. McKee and Woolcott (1949) reported that individuals exposed to 0.062 mg GB/m<sup>3</sup> for 20 minutes per day exhibited no signs of toxicity the first three days; however, miosis appeared after the fourth day of exposure. The 1-hour no-effect level would be 0.02 mg/m<sup>3</sup>. Using the relative potency approach (see Appendix G), the equivalent concentrations for GA and GD are 0.05 mg/m<sup>3</sup> and 0.013 mg/m<sup>3</sup>, respectively.

For HD, a Ct of 12 mg-min/m<sup>3</sup> is considered a no-effect dose for eye irritation at ambient temperatures (McNamara et al., 1975). The maximum allowable Ct for skin effects is 5 mg-min/m<sup>3</sup> and that for eye effects is 2 mg-min/m<sup>3</sup> (DA, 1974, 1992). Minimum effect levels for exposure to Lewisite vapors were not found in the available literature.

### 1.3.9 Multiple Chemical Exposures

HBESLs are calculated for single compounds, and USEPA does not have an established method for deriving screening values for chemical mixtures. For contaminants with similar modes of action and/or identical target organs, the sum total of all exposures from such chemicals is often evaluated in the baseline risk assessment for the site. For screening assessments, several approaches may be used to evaluate multiple chemical exposures. The sum total of the concentrations of all contaminants in a specific medium (i.e., soil or water) having a similar toxic effect may be compared with the lowest HBESL for that medium. This would be a conservative approach, with a relatively large margin of safety. A second approach might be to develop a hybrid HBESL based on the relative toxicity and media concentration of each of the contaminants having a similar mode of action.

### 1.3.10 Ecological Impacts

The HBESLs that are currently used by USEPA do not consider potential ecological impacts. The HBESLs may or may not be protective of certain habitats and species. Further investigation of this issue may be warranted in some cases. USEPA has developed guidelines for assessing ecological risks from chemical contaminants (USEPA, 1996e). Furthermore, a method exists for deriving ecological benchmarks, similar to HBESLs, for screening sites for potential ecological effects. This method utilizes toxicological data to establish screening values that are intended to be protective of wildlife populations rather than individual organisms (Sample et al., 1996; Suter and Tsao, 1996). This method has been applied to military-unique compounds such as RDX and TNT (Talmage et al., 1999) and could also be used with the chemical warfare agents.

## **2. EXPOSURE ASSESSMENT**

### **2.1 EXPOSURE SCENARIOS**

HBESLs in this document have been established to generically describe different types of situations that may result in human exposure to chemical agent residue as an environmental contaminant. The generic situations include a commercial/industrial scenario and a residential scenario. The scenarios are the same standard scenarios used by the EPA in calculating their industrial/agricultural compound screening levels. These scenarios may be used to establish screening goals for cleanups conducted at Department of Defense/Army facilities/sites. Choosing the scenario that best describes a given situation/site is the first step to attributing decisions to site-specific data. For instance, the HBESL for a residential exposure scenario may be exceeded, but if the future use of the site clearly does not indicate a residential setting, then comparing contaminant concentrations for the industrial/commercial scenario may be more appropriate. Careful selection of an initial screening level can avoid delays or unnecessary expenditures. Multi-scenario HBESLs provide a quick, efficient screening tool that still offers a certain degree of site-specific information.

#### **2.1.1 Commercial/Industrial Scenario**

Following cleanup and environmental restoration activities, a site might be used for commercial or industrial businesses, at which time individuals may be exposed to residual amounts of the contaminants. The potential for exposure is highly dependent on whether the individuals come into direct contact with the soil. If development of the site involves capping the soil with an impervious material such as concrete or asphalt, then contact will be minimized. If extensive areas of surface soils remain exposed, then the potential for exposure will be greater, and if the site is subject to excavation activities, then the potential exposure will be at a maximum. Both the PRGs used by USEPA Region IX and the RBCs used by USEPA Region III include an industrial/commercial scenario for potential exposure to contaminated soil. The basic exposure pathways and parameters used by these USEPA regions will also be used here. The Soil Screening Level approach (SSL) does not include the industrial scenario.

#### **2.1.2 Residential Scenario**

The residential scenario considers two possibilities: 1) that residential populations currently living near the site might be exposed as a result of environmental transport of the contaminants offsite; and 2) that the site itself might be used as a residential development at some future time after environmental restoration activities have been completed. Because residence times at a single location may be for many years, the screening values developed for residential scenarios are designed to be very protective (i.e., 30-year exposure duration). There are unique military situations, such as on-post housing, which would include residential exposures; however, because residence times for military personnel at a given installation are limited, it

would be expected that the screening levels developed for the general public would also be protective of military dependents living near the sites.

### **2.1.3 Other Scenarios**

The two described scenarios are the basis for general screening levels, with the residential scenario levels used most often as a “first cut” and industrial levels considered on a site-specific basis or as preliminary remediation goals (USEPA 1998). However, with limitations, there are additional applications of the chronic risk screening methodology. Other ‘types’ of scenarios that may require an assessment to evaluate risk associated with a chronic chemical exposure include ‘trespasser’ scenarios- individuals who, on occasion, unknowingly or inappropriately (often illegally) enter an area of contamination concern but where no other population is involved, and agricultural land use. These types of scenarios and potential use of the EPA models are evaluated in Appendices C and D. Where data were identified and deemed reasonable for assumptions applicable to these scenarios (i.e. trespasser scenario), the assumptions and rationale are described and example HBESLs are calculated. Where no reasonable data could be ‘fit’ or where a generic scenario could not be defined (such as for agricultural scenarios), a discussion of considerations and uncertainties is provided. In each scenario, the uncertainties and limitations of use of the model are discussed.

## **2.2 EXPOSURE PATHWAYS**

For the industrial scenario, the pathways of greatest concern would be dependent on the type of work involved and the degree to which contaminated soil has been isolated from the work areas. High potential exposures from skin contact, inadvertent ingestion, and inhalation of volatiles or particulates might be expected for unprotected excavation workers at unimproved sites. In contrast, relatively low exposure, mainly from inhalation of volatiles, might occur at sites that have been largely paved over.

In a residential setting, inadvertent ingestion of soil and skin contact with soil may be significant exposure pathways, particularly for children in geographic regions with mild climates which allow for a considerable amount of time spent outside the home each day. Inhalation of volatiles and fugitive dust are also possible exposure pathways; the magnitude of the exposure by each pathway being dependent on whether the contamination is in surface or subsurface soils.

## **2.3 EXPOSURE PARAMETERS**

The exposure scenarios and pathways discussed above require the use of various parameters that may be population-, chemical- or site-specific. Population-specific parameters are dependent on age, body size (body surface area), soil ingestion rates, and activity patterns of the individuals who may be exposed. These factors determine the frequency and extent of the exposure. The type of soil at a site determines the

amount of agent adsorbed to soil particles. Soil type also affects how strongly the soil adheres to the skin and, consequently, how much chemical is available for absorption through the skin. The physical-chemical characteristics of the compound, the area of the body exposed, and the ambient temperature also affect the rate of absorption through the skin. Physical and chemical characteristics of the individual contaminants (i.e., volatility) also determine the extent that a chemical will be transported from one environmental medium to another (i.e., from soil to air). These factors, in turn, will determine whether a specific exposure pathway is relevant in deriving environmental screening levels.

In the screening approaches discussed in this report, USEPA default values are used for many of the population-, chemical-, or site-specific parameters. These default values are those recommended by USEPA's OSWER for SSLs, USEPA Region III for RBCs, USEPA Region IX for PRGs, and by USEPA Region IV. Table 2-1 lists these values, which represent estimates of average or maximum values. For a given parameter, the 50th percentile is considered by USEPA to be the average exposure level (i.e., 50% of the population would have an inhalation rate equal to or less than the amount), and the 90th or 95th percentile is considered by USEPA to be the upper bound or "reasonable maximum exposure (RME)" (i.e., 90% or 95% of the population would have an inhalation rate equal to or less than the amount) (USEPA, 1989a). In screening assessments, USEPA uses 50th percentiles for some parameters and RMEs for others.

The following sections discuss the individual parameters (population-, chemical- and site-specific). The default values, as well as alternatives, are evaluated and a rationale is provided for the value(s) chosen for the calculations in this report. It should be noted that many of the default values used by USEPA were originally recommended in the Exposure Factors Handbook (USEPA, 1989a). The handbook has been revised and updated (USEPA, 1997d), and changes are being recommended in some of the default values, but these have not been officially adopted by the USEPA for Superfund risk assessments. There are also other sources of parameter values, including regional and state guidelines, open literature values, and defaults used by organizations such as the American Industrial Health Council (AIHC, 1994). Non-USEPA default values are generally not discussed in this report, except for those parameters that have no current USEPA-recommended default.

<b>Table 2-1. USEPA and regional default values for risk assessment calculations</b>				
<b>Parameter</b>	<b>Region III (RBCs)</b>	<b>Region IX (PRGs)</b>	<b>OSWER (SSLs)</b>	<b>Region IV</b>
Body weight - adult (BW <sub>a</sub> )	70 kg	70 kg	70 kg	
Body weight - children (BW <sub>c</sub> )	15 kg	15 kg	15 kg	
Body weight - adolescent trespasser (BW <sub>t</sub> )	-	-	-	45 kg
Averaging time - carcinogens (AT <sub>c</sub> )	25,550 d	25,550 d	25,550 d	
Averaging time - noncarcinogens, residential, industrial (AT <sub>n</sub> )	365 x ED	365 x ED	365 x ED	
Exposure frequency - residential (EF <sub>r</sub> )	350 d/yr	350 d/yr	350 d/yr	350 d/yr
Exposure frequency - industrial (EF <sub>i</sub> )	250 d/yr	250 d/yr	-	250 d/yr
Exposure duration - residential (ED <sub>r</sub> ) (for water contaminants)	30 yr	30 yr	30 yr	30 yr
Exposure duration - residential, child (ED <sub>c</sub> ) (for soil contaminants)	6 yr	6 yr	6 yr	6 yr
Exposure duration - industrial (ED <sub>i</sub> )	25 yr	25 yr	-	25 yr
Exposure duration - adolescent trespasser (ED <sub>t</sub> )	-	-	-	10 yr
Tapwater ingestion - adult (IRW <sub>a</sub> )	2 L/d	2 L/d	2L/d	2 L/d
Tapwater ingestion - child (IRW <sub>c</sub> )	1 L/d	1 L/d	-	1 L/d
Tapwater ingestion factor (IFW <sub>adj</sub> )	1.09 L-yr/ kg-d	1.1 L-yr/ kg-d	-	-
Soil ingestion - adult, residential (IRS <sub>a</sub> )	100 mg/d	100 mg/d	-	100 mg/d
Soil ingestion - adult, industrial (IRS <sub>i</sub> )	50 <sup>a</sup> mg/d	50 mg/d	-	50-480 mg/d
Soil ingestion - child (IRS <sub>c</sub> )	200 mg/d	200 mg/d	200 mg/d	200 mg/d
Soil ingestion factor (IFS <sub>adj</sub> )	114.29 mg- yr/kg-d	114 mg- yr/kg-d	114 mg- yr/kg-d	
Soil contact factor (SFS <sub>adj</sub> )	-	504 mg- yr/kg-d	-	-
Inhalation rate - adult (IRA <sub>a</sub> )	20 m <sup>3</sup> /d	20 m <sup>3</sup> /d	-	20 m <sup>3</sup> /d
Inhalation rate - child (IRA <sub>c</sub> )	12 m <sup>3</sup> /d	10 m <sup>3</sup> /d	-	15 m <sup>3</sup> /d
Inhalation rate - industrial (IRA <sub>i</sub> )	-	-	-	20 m <sup>3</sup> /d

<b>Table 2-1. USEPA and regional default values for risk assessment calculations</b>				
<b>Parameter</b>	<b>Region III (RBCs)</b>	<b>Region IX (PRGs)</b>	<b>OSWER (SSLs)</b>	<b>Region IV</b>
Inhalation factor ( $IFA_{adj}$ , $InhF_{adj}$ )	11.66 m <sup>3</sup> - yr/kg-d	11 m <sup>3</sup> -yr/kg- d	-	-
Exposed skin surface - adult ( $SA_a$ )	-	5700 cm <sup>2</sup>	-	-
Exposed skin surface - child ( $SA_c$ )	-	2900 cm <sup>2</sup>	-	-
Volatilization Factor for tapwater ( $VF_w$ )	0.5 L/m <sup>3</sup>	0.5 L/m <sup>3</sup>		-
Volatilization Factor for soil ( $VF_s$ )	chem. spec.	chem. spec.	chem. spec.	chem. spec.
Particulate Emission Factor for soil (PEF)	1.32 x 10 <sup>9</sup> m <sup>3</sup> /kg	1.32 x 10 <sup>9</sup> m <sup>3</sup> /kg	1.32 x 10 <sup>9</sup> m <sup>3</sup> /kg	-
Dermal Absorption Factor ( $ABS_{derm}$ ) organics inorganics	-	10% 1%	-	1% 0.1%
GI Absorption Factor ( $ABS_{gi}$ ) volatiles semivolatiles nonvolatiles	NA	NA	NA	80% 50% 20%
Soil-to-Skin Adherence Factor - child ( $AF_c$ )	-	0.3 mg/cm <sup>2</sup>	-	1.0 mg/cm <sup>2</sup> (RME)
Soil-to-Skin Adherence Factor - adult ( $AF_a$ )	-	0.08 mg/cm <sup>2</sup>	-	

Sources: USEPA, 1996a; 1996d; 1998

<sup>a</sup> For industrial land use scenarios, USEPA Region III uses 0.5 as the fraction of ingested soil that is contaminated.

### 2.3.1 Population-Specific Parameters

#### 2.3.1.1 Age and body weight (BW)

The USEPA default value for adult BW is 70 kg. A new default value of 71.8 kg has been proposed in the Exposure Factors Handbook (USEPA, 1997d); however, this value has not yet been adopted by the OSWER. For children 1-6 years old, the group considered by USEPA to be the most susceptible to ingestion of contaminated soil, an average BW of 16 kg is the recommended default in RAGS; however, for PRGs,

RBCs and SSLs, a default value of 15 kg is used. The Exposure Factors Handbook (USEPA, 1997d) gives age-specific BWs for children, but does not recommend a single value for children 1-6 years old.

In this report, BWs of 70 kg for adults and 15 kg for children are used.

#### 2.3.1.2 Averaging Time (AT<sub>c</sub>) for Carcinogens

In the derivation of screening levels for carcinogens, USEPA uses a standard default life span of 70 years, and this USEPA value is also used in the calculations made in this report. The Exposure Factors Handbook (USEPA, 1997d) recommends that 75 years be used for the average life expectancy of the general population; however, this value has not been officially adopted by USEPA. In the screening methods discussed in this report, the averaging time for noncarcinogens is equivalent to the exposure duration (see below).

In this report, an average life span of 70 years is used to calculate cancer risks.

#### 2.3.1.3 Exposure time (ET), exposure duration (ED) and exposure frequency (EF)

The average daily exposure to a chemical contaminant is a function of the EF (in days per year) multiplied by the ED (in years) divided by the total number of days over which the exposure occurs. In USEPA baseline and screening risk assessments, the ED is considered to be equivalent to the averaging time for noncarcinogenic endpoints. If an exposure exceeds a minimum duration defined as chronic (i.e., 7 years according to USEPA), the potential for chronic effects, as defined by the chronic RfD, will remain regardless of the length of any subsequent nonexposure period.

The standard USEPA default used for ED for occupational exposures is 25 years and, based on a 5-day work week, the standard default for EF is 250 days/year (this value excludes the 10 working days covered by a 2-week vacation period).

In this report, the EF and ED parameters used for occupational scenarios are 250 days/year and 25 years, respectively.

For residential scenarios, ED is determined by the number of years of occupancy at the same residence. For baseline risk assessments, the USEPA default values for residence time are 9 years for a median value and 30 years for an upper bound estimate (50th and 90th percentiles, respectively) (USEPA, 1989a). PRGs, RBCs, and SSLs are based on the upper bound estimate of 30 years. It should be noted that, in risk assessments for carcinogens, the 30-year residency period is assumed to occur from birth to age 30, and calculations of intake rates are based on time-weighted averages (TWAs). The upper bound default value for EF for a residential scenario is 350 days/year (this value excludes a 2-week per year vacation period during which time it is assumed that no exposure will occur).

In this report, the EF and ED parameters used for residential scenarios are 350 days/year and 30 years, respectively.

#### 2.3.1.4 Skin contact with contaminated soil (SA)

For exposures that may occur as a result of skin contact with contaminated soil, the magnitude of exposure is dependent on the amount of skin surface area exposed. The area of skin exposed is a function of the age, body size, clothing worn, and activity pattern of the individual. Thus, for specific scenarios only certain body parts may be exposed (body part surface areas are given in Table 2-2). USEPA has suggested that for most soil contact scenarios for adults, the hands, lower legs, forearms, neck and head would be exposed and that the exposure would be equivalent to 25% of the total body surface area (USEPA, 1992). The default values *currently* used by USEPA Region IX (USEPA 1998) are 5700 cm<sup>2</sup> for adults and 2900 cm<sup>2</sup> for children. Body surface area estimates for children 2-10 years old are shown in Table 2-2.

In this report, exposed skin surface areas of 5700 cm<sup>2</sup> for adults and 2900 cm<sup>2</sup> for children are used.



<b>Table 2-2. Body surface areas for 50th percentile of population (m<sup>2</sup>)</b>								
<b>Age (yr)</b>	<b>Total body</b>		<b>Body part surface area for males</b>					
	<b>Male</b>	<b>Female</b>	<b>Arms</b>	<b>Hands</b>	<b>Legs</b>	<b>Feet</b>	<b>Head</b>	<b>Trunk</b>
2 < 3	0.603 (6030 cm <sup>2</sup> )	0.579 (5790 cm <sup>2</sup> )						
3 < 4	0.664 (6640 cm <sup>2</sup> )	0.649 (6490 cm <sup>2</sup> )	0.096 (960 cm <sup>2</sup> )	0.040 (400 cm <sup>2</sup> )	0.18 (1800 cm <sup>2</sup> )			
4 < 5	0.731 (7310 cm <sup>2</sup> )	0.706 (7060 cm <sup>2</sup> )						
5 < 6	0.793 (7930 cm <sup>2</sup> )	0.779 (7790 cm <sup>2</sup> )						
2 < 6	0.698 (6980 cm <sup>2</sup> )	0.678 (6780 cm <sup>2</sup> )						
2 < 6	0.688 (6880 cm <sup>2</sup> )							
3 < 10	0.866 <sup>a</sup> (8660 cm <sup>2</sup> )	0.851 <sup>a</sup> (8510 cm <sup>2</sup> )	0.116 <sup>b</sup> (1160 cm <sup>2</sup> )	0.047 <sup>b</sup> (470 cm <sup>2</sup> )	0.239 <sup>b</sup> (2390 cm <sup>2</sup> )	0.0627 <sup>b</sup> (627 cm <sup>2</sup> )	0.114 <sup>b</sup> (1140 cm <sup>2</sup> )	0.287 <sup>b</sup> (2870 cm <sup>2</sup> )
Adult	1.94 (19,400 cm <sup>2</sup> )	1.69 (16,900 cm <sup>2</sup> )	0.228 <sup>c</sup> (2280 cm <sup>2</sup> )	0.084 <sup>c</sup> (840 cm <sup>2</sup> )	0.505 <sup>c</sup> (5050 cm <sup>2</sup> )	0.112 <sup>c</sup> (1120 cm <sup>2</sup> )	0.118 <sup>c</sup> (1180 cm <sup>2</sup> )	0.569 <sup>c</sup> (5690 cm <sup>2</sup> )

**Sources:** USEPA, 1989a, 1989b, 1992

<sup>a</sup>Calculated as an average of the median values for four age groups as given in USEPA, 1989a

<sup>b</sup>Calculated from the percentage of total body surface area for each body part

<sup>c</sup>Mean values (USEPA, 1989a)

### 2.3.1.5 Soil ingestion rates (IR<sub>s</sub>)

Total exposures resulting from ingestion of soil are dependent on age-specific ingestion rates, EF and ED, and on the fraction of soil ingested from the contaminated source.

Children 1-6 years old are the group most susceptible to ingestion of soil (USEPA, 1989a). For this group, 200 mg/day is considered a typical soil consumption rate (50th percentile) and 800 mg/day is a "reasonable worst-case value" (90th percentile) (USEPA, 1989a). The default value used for PRGs, RBCs, and SSLs is 200 mg/day for children 1-6 years old. The new Exposure Factors Handbook (USEPA, 1997d) recommends a new mean value of 100 mg/day, and an upper percentile value of 400 mg/day; however, these values have not yet been adopted by USEPA.

Although information on soil ingestion rates for individuals over 6 years old is very limited (USEPA, 1989a), the default value used for PRGs, RBCs, and SSLs is 100 mg/day. The new Exposure Factors Handbook (USEPA, 1997d) recommends an adult soil ingestion default value of 50 mg/day.

Another factor that may be included or incorporated into the soil ingestion rate is the fraction of soil ingested (FS) that is contaminated. The fraction of soil ingested from a contaminated source is dependent on the activity patterns of the individuals who may be exposed. Children may come in contact with the contaminated soil in their residential neighborhood, but perhaps not with contaminated soil at school, or just the opposite scenario may occur. For screening level calculations, the assumption is made that for residential exposures, all of the soil ingested comes from the contaminated source. For occupational exposures, USEPA Region III uses the assumption that the fraction of soil ingested from the contaminated source is 0.5. Applied to an ingestion rate of 100 mg/day, this results in a daily intake 50 mg/day (USEPA, 1996a). USEPA Region IX uses an occupational soil ingestion rate of 50 mg/day without incorporating a FS value (USEPA, 1998). Though the value of 50mg/day is a default value for the occupational scenario, available data (USEPA, 1997d) suggests that for very specific occupational exposures, such as excavation workers, higher defaults for soil ingestion may be appropriate.

It is also a consideration that exposure frequency for the soil ingestion pathway depends on the number of days during which soil ingestion may occur, and this, in turn, depends on climate and individual behavior patterns. USEPA has estimated that "ingestion of contaminated soil could occur typically 75% of the time over a 3-year period. In a "reasonable worst-case," this would occur 100 percent over a 6-year period" (USEPA, 1989a). USEPA exposure frequency defaults are 40-350 events per year (central and upper bound estimates). The latter value presumably would be appropriate in tropical or subtropical regions where children may be outdoors year round.

In this report, the assumption is that 100% of soil ingested by a child is contaminated, resulting in a total contaminated soil ingestion rate of 200 mg/day. For residential adults the rate is 100mg/day. For occupational exposures, the amount of contaminated soil ingested is assumed to be 50 mg/day.

### 2.3.1.6 Inhalation rates (IR)

The standard USEPA default for inhalation rate is 20 m<sup>3</sup> per day for adults. The new Exposure Factors Handbook (USEPA, 1997d) recommends an inhalation default value of 15.2 m<sup>3</sup> per day for adult men and 11.3 m<sup>3</sup> per day for adult women; a single general population value is not given. USEPA Region III uses an inhalation rate of 12 m<sup>3</sup>/day for children, whereas Region IX uses an inhalation rate of 10 m<sup>3</sup>/day for children. The Exposure Factors Handbook recommends age-specific inhalation rates for children: 6.8 m<sup>3</sup>/day for 1-2 year olds; 8.3 m<sup>3</sup>/day for 3-5 year olds; and 10 m<sup>3</sup>/day for 6-9 year olds.

In this report, an inhalation rate of 20 m<sup>3</sup> is used adults and 10 m<sup>3</sup>/day is used for children.

## 2.3.2 Chemical-Specific Parameters

Chemical-specific parameters used in deriving HBESLs for the chemical warfare agents are listed in Table 2-3. Several of these parameters are discussed in more detail in the following sections.

### 2.3.2.1 Gastrointestinal absorption factor (ABS<sub>gi</sub>)

Gastrointestinal absorption factors (ABS<sub>gi</sub>) are used to estimate a dermal RfD from an oral RfD. The dermal RfD is then compared with estimated exposures through skin contact with contaminated soil. Gastrointestinal absorptions factors are not readily available for many compounds, and USEPA Region IX allows the use of oral toxicity values (RfDs and slope factors) in place of estimates of dermal toxicity values. USEPA Region IV recommends using default gastrointestinal absorption values of 80% for volatile organics, 50% for semivolatile organics, and 20% for inorganics (USEPA, 1995b). USEPA Region IV does not provide guidance for differentiating between volatile and semivolatile organic compounds.

In this report, oral toxicity values are used for dermal pathways except for Lewisite, where available dermal toxicity data were used to establish a more appropriate dermal toxicity value [discussed in detail in the Lewisite chapter (Chapter 9) and in section 1.2].

Table 2-3. Chemical/environmental parameters for chemical agents						
Parameter	HD	L	GA	GB	GD	VX
Vapor pres. (mm Hg at 25°C)	0.11	0.58	0.07	2.9	0.40	0.0007
Solubility (g/L)	0.920	0.5	98	miscible	21	10 - 50 <sup>i</sup>
Henry's Law Constant (H) (atm·m <sup>3</sup> /mol)	2.1 x 10 <sup>-5</sup> <sup>a</sup>	3.2 x 10 <sup>-4</sup> <sup>g</sup>	1.5 x 10 <sup>-7</sup> <sup>g</sup>	5.34 x 10 <sup>-7</sup> <sup>a</sup>	4.56 x 10 <sup>-6</sup> <sup>g</sup>	3.5 x 10 <sup>-9</sup> <sup>a</sup>
Dimensionless Henry's Law Constant (H') <sup>f</sup>	8.6 x 10 <sup>-4</sup>	1.3 x 10 <sup>-2</sup>	6.15 x 10 <sup>-6</sup>	2.2 x 10 <sup>-5</sup>	1.87 x 10 <sup>-4</sup>	1.43 x 10 <sup>-7</sup>
Liquid density (g/mL at 25°C)	1.27	1.88	1.08	1.09	1.02	1.0083
Air diffusivity (cm <sup>2</sup> /s)	0.099	0.099	0.092	0.10	0.082	0.062
Water diffusivity (cm <sup>2</sup> /s)	8.4 x 10 <sup>-6</sup>	9.0 x 10 <sup>-6</sup>	7.5 x 10 <sup>-6</sup>	8.2 x 10 <sup>-6</sup>	6.8 x 10 <sup>-6</sup>	5.3 x 10 <sup>-6</sup>
Apparent diffusivity (cm <sup>2</sup> /s)	5.0 x 10 <sup>-6</sup>	NA <sup>h</sup>	2.35 x 10 <sup>-7</sup>	5.4 x 10 <sup>-7</sup>	5.57 x 10 <sup>-7</sup>	1.7 x 10 <sup>-8</sup>
Volatilization factor (m <sup>3</sup> /kg)	5.62 x 10 <sup>4</sup>	NA <sup>h</sup>	2.6 x 10 <sup>5</sup>	1.7 x 10 <sup>5</sup>	1.7 x 10 <sup>5</sup>	9.67 x 10 <sup>5</sup>
Soil saturation limit (mg/kg)	460	NA <sup>h</sup>	32,438	-	31,585	6500
log K <sub>ow</sub>	1.37 <sup>a</sup>	NA <sup>h</sup>	0.384 <sup>b</sup>	0.299 <sup>b</sup>	1.82 <sup>b</sup>	2.09 <sup>a</sup>
log K <sub>oc</sub> <sup>d</sup>	2.12	NA <sup>h</sup>	1.59	1.54	2.37	2.51
K <sub>oc</sub>	133	NA <sup>h</sup>	38.5	34.6	234	327
K <sub>d</sub> <sup>e</sup>	0.798	NA <sup>h</sup>	0.231	0.208	1.404	1.962

SOURCES: DA, 1974, unless otherwise noted: for most values data points are for 20-25°C

<sup>a</sup> Value from Small, 1984

<sup>b</sup> Experimental value; see Appendix H

<sup>c</sup> Due to rapid hydrolysis, water solubility data are virtually meaningless (Rosenblatt et al., 1975)

<sup>d</sup> Estimated using the regression equation:  $\log K_{oc} = 1.377 + 0.544 \log K_{ow}$  (see Lyman et al., 1982, Equation 4-8).

<sup>e</sup>  $K_d = K_{oc} \times f_{oc}$ , where  $f_{oc}$  = organic carbon in soil (0.006 g/g, USEPA Region IX default for PRGs)

<sup>f</sup>  $H' = 41 \times \text{Henry's Law Constant}$  (USEPA, 1996)

<sup>g</sup>  $H = H^* \times RT$ ;  $H^*$  = ratio of the volatility and solubility; R = gas constant ( $8.2 \times 10^{-5}$  atm·m<sup>3</sup>/mol·K); and T = temperature in K (20°C = 293.15°K)

<sup>h</sup> Cannot be calculated due to rapid degradation

<sup>i</sup> MacNaughton and Brewer, 1994

### 2.3.2.2 Dermal absorption factor ( $ABS_{\text{derm}}$ )

The dermal absorption factor ( $ABS_{\text{derm}}$ ) is a chemical-specific value which allows for the estimation of the absorbed dose. A default value for skin absorption has not been adopted agency-wide by USEPA. The Soil Screening Guidance Document (USEPA, 1996c) indicates that absorption via the dermal route must be greater than 10% to equal or exceed ingestion exposures (assuming 100% absorption of the chemical via the gastro-intestinal tract). Of 110 compounds evaluated by USEPA, only pentachlorophenol had a dermal absorption greater than 10%. However, it was also reported that certain semivolatile organic compounds such as BaP may be of concern through this exposure route (USEPA, 1996c).

For volatile organics such as benzene and 1,1-dichloroethane and other compounds having a vapor pressure similar to or greater than that of benzene (i.e., 95.2 mm Hg), USEPA Region III recommends using a default skin absorption factor of 0.05% (USEPA, 1995a). For volatile compounds with a lower vapor pressure, USEPA Region III recommends a default of 3%. Region III recommends a default value of 10% for semivolatile organics, and gives BaP as an example; however, the vapor pressure of BaP is only  $5 \times 10^{-9}$  mm Hg, indicating a very low potential for volatilization. For calculating PRGs, USEPA Region IX uses a default value of 10% for organics and 1% for inorganics (with the exception that an absorption factor of 3% is used for inorganic arsenic) (USEPA, 1998).

Although experimental data indicate that the skin absorption rates for many semivolatile organic compounds range from 1-10% for the pure compound, much lower absorption rates are likely to occur when the chemical is bound to soil particles. For this reason, USEPA Region IV recommends 1% as the default for organic compounds and 0.1% for inorganics (USEPA, 1995b).

Dermal absorption data for the chemical warfare agents are listed in Table 2-4. Absorption of pure agent VX on the forearm and cheek ranged from about 2 to 20% in tests conducted at 18°C (Craig et al., 1977). Lower values would be expected for the more volatile G agents, as shown by a skin absorption rate of less than 1% for the volatile nerve agent GB (Marzulli and Williams, 1953).

Based on soil partitioning coefficients, water solubility and flux across the skin, Major (1998) estimated the theoretical rates of dermal absorption of agents HD, GA, GD, GB, and VX from a soil matrix (see Appendix H). Because the HBESL exposure scenarios focus on dermal contact with contaminated soil, the  $ABS_{\text{derm}}$  values calculated by Major are used in this report. Because dermal absorption is possible until the soil is removed from the skin, cumulative absorption rates are used in the HBESL calculations. It was conservatively assumed that for a residential scenario the soil might remain on the skin for as long as 12 hours. For the commercial/industrial scenario an 8-hour cumulative absorption was used to coincide with the 8-hour occupational exposure duration.

An experimentally-derived  $ABS_{\text{derm}}$  was not available for Lewisite; therefore, a default value of 0.1 is used in accordance with USEPA Region IX guidelines for organic compounds (USEPA 1998).

**Table 2-4. Dermal absorption values for chemical agents**

ABS <sub>derm</sub> values used in this report for soil-bound agents are:		
<u>Agent</u>	<u>Residential</u>	<u>Commercial/industrial</u>
HD	8.4%/12 hr	5.6%/8 hr
Lewisite	10%/day	10%/day
GA	3.1%/12 hr	2.1%/8 hr
GB	4.2%/12 hr	2.8%/8 hr
GD	9.4%/12 hr	6.1%/8 hr
VX	3.3%/12 hr	2.2%/8 hr

### 2.3.2.3 Volatilization factor for soil (VF<sub>s</sub>)

Volatilization of a chemical from soil is a function of the concentration of the chemical, the density of the soil particles, and the rate of diffusion of the chemical from the soil to air. Appendix A provides an equation for deriving the VF<sub>s</sub> for each chemical agent. Derivation of the diffusion coefficient for each agent requires five chemical-specific parameters: Henry's Law Constant, diffusivity coefficient for air, diffusivity coefficient for water, soil-water partition coefficient, and soil organic carbon-water partition coefficient. The values for these parameters for each chemical agent are calculated in Appendix A and listed in Table 2-3. They are discussed further in the following sections. If a chemical is not volatile by the USEPA's definition of volatility, volatilization is not considered a potential exposure pathway; however, in the derivation of screening values the VF<sub>s</sub> is replaced with a Particulate Emission Factor (PEF, see Section 2.3.3.2) which takes into account the possibility that exposures may occur as a result of inhalation of contaminated airborne particles.

**Henry's Law Constant (H).** This constant is a ratio of the volatility of a chemical to its water solubility, and thus is a measure of the tendency of a chemical to volatilize from water. Henry's Law Constants can be determined experimentally or estimated from the vapor pressure and water solubility of the chemical. Methods for estimating Henry's Law Constants for the chemical warfare agents are given in Appendix A. Henry's Law Constants for the chemical agents are listed in Table 2-3. As recommended by USEPA, the Henry's Law Constant was used not only to calculate the VF<sub>s</sub> for each agent, but also to determine whether volatilization would be a significant exposure pathway. According to USEPA, chemicals having an H value of greater than  $1 \times 10^{-5}$  atm-m<sup>3</sup>/mol and a molecular weight of less than 200 are likely to represent an inhalation hazard as a result of volatilization from water or soil. Based on this definition, only

HD is considered to be sufficiently volatile to require the inclusion of the inhalation pathway in the exposure assessment.

Based on USEPA's definition of volatility, only HD is considered to be subject to volatilization from soil.

**Diffusivity in Air ( $D_a$ )**. This coefficient is a measure of the tendency of a chemical to diffuse through air. It can be determined experimentally or estimated from information on the molecular weight and liquid density of a chemical. Derivations of the air diffusivity coefficients for the chemical warfare agents are given in Appendix A and listed in Table 2-3.

**Diffusivity in Water ( $D_w$ )**. This coefficient is a measure of the tendency of a chemical to diffuse through water. It can be determined experimentally or estimated from the molar volume of a chemical. Derivations of the water diffusivity coefficients for the chemical warfare agents are given in Appendix A and listed in Table 2-3.

**Soil Organic Carbon-Water Partition Coefficient ( $K_{oc}$ )**. This coefficient is a measure of the tendency of a chemical to partition between water and soil organics. The  $K_{oc}$  can be derived from a chemical's octanol-water partition coefficient ( $K_{ow}$ ) using the following equation (see Lyman et al., 1982).

$$\log K_{oc} = 1.377 + \log K_{ow} \quad (2-1)$$

Chemical-specific  $K_{ow}$  values were obtained from the available literature (see Table 2-3).  $K_{oc}$  values for the chemical warfare agents were derived from  $K_{ow}$  values using Equation 2-1 and are also listed in Table 2-3.

**Soil-Water Partition Coefficient ( $K_d$ )**. This coefficient is a measure of the tendency of a chemical to bind to soils. It is derived by multiplying the soil organic carbon-water partition coefficient ( $K_{oc}$ ) by the fraction of organic carbon in the soil ( $f_{oc}$ ).

$$K_d = K_{oc} \times f_{oc} \quad (2-2)$$

The default  $f_{oc}$  used by OSWER (for inhalation of volatiles), as well as by USEPA Region IX for calculating apparent diffusivities, is 0.006 g/g.  $K_d$  values for the chemical warfare agents, as derived from Equation 2-2, are presented in Table 2-3.

#### 2.3.2.4 Soil saturation limit ( $C_{\text{sat}}$ )

The soil saturation limit ( $C_{\text{sat}}$ ) of a chemical is used to determine the concentration of a chemical in soil below which volatilization is a function of the solubility, volatility, and diffusivity of the chemical. Above this limit the chemical will also exist in soil in the pure undissolved state. Screening levels incorporating a volatilization factor are not accurate for chemical concentrations in soil above the  $C_{\text{sat}}$ . The equation for deriving  $C_{\text{sat}}$  values is given in Appendix A. Soil saturation limits for the chemical agents are listed in Table 2-3.

### 2.3.3 Site-Specific Parameters

#### 2.3.3.1 Soil-to-skin adherence factor (AF)

The type of soil at a given site determines the soil-to-skin adherence factor (AF). In the absence of site-specific data, the Superfund Guidance Document recommends using the following default values: 1.45 mg/cm<sup>2</sup> for commercial potting soil and 2.77 mg/cm<sup>2</sup> for kaolin clay (USEPA, 1989b). USEPA (1992) has more recently reported that "a range of values from 0.2 mg/cm<sup>2</sup> to 1.5 mg/cm<sup>2</sup> per event appear possible." Based on the recently developed Dermal Exposure Guidelines, USEPA Region IX now uses a soil adherence value of 0.08 mg/cm<sup>2</sup> for PRG calculations for adults and 0.3 mg/cm<sup>2</sup> for children (USEPA, 1998). Because the USEPA Region IX approach is the one that is most commonly used, the same defaults will be used in this report.

In this report, a soil-to-skin adherence factor of 0.08 mg/cm<sup>2</sup> is used for adults and 0.3 mg/cm<sup>2</sup> is used for children.

#### 2.3.3.2 Particulate emission factor (PEF)

Inhalation of fugitive dusts is an exposure pathway that is considered in deriving PRGs and SSLs. Since the screening level derived for ingestion of soil is usually several orders of magnitude lower than the fugitive dust pathway, the fugitive dust pathway does not need to be routinely considered for organic chemicals in surface soils (USEPA, 1996c). Derivation of a fugitive dust SSL requires calculation of a PEF that relates the concentration of the chemical in soil to its concentration in dust particles in air. The PEF represents an annual average emission rate based on wind erosion. Derivation of the PEF is given in Appendix A. The default PEF used by USEPA is  $1.32 \times 10^9$  m<sup>3</sup>/kg (USEPA, 1998).

In this report, a default PEF of  $1.32 \times 10^9$  m<sup>3</sup>/kg is used.



### 3. METHODS FOR DERIVING ENVIRONMENTAL SCREENING LEVELS

This chapter describes the equations for calculating Risk-Based Concentrations (RBCs), Preliminary Remediation Goals (PRGs), and Soil Screening Levels (SSLs).

#### 3.1 RISK-BASED CONCENTRATIONS (RBCs)

Risk-based concentrations have been developed by USEPA Region III (USEPA, 1996a). Current EPA Region III models are used to estimate RBCs for exposure to residential tapwater, ambient air, consumption of edible fish, and residential and industrial soils. For the chemical warfare agents, RBCs are estimated in this report only for residential and industrial soil. The parameters used in the RBC equations are listed in Table 3-1. The abbreviations are those used by USEPA Region III (USEPA, 1996a).

**3.1.1 RBC for Residential Soil - Noncancer Endpoint.** A residential soil RBC for a noncancer endpoint for residential soil is derived using the following equation (USEPA, 1996a):

$$RBC_s = \frac{THQ \times RfDo \times BWc \times ATn}{Efr \times EDc \times \left( \frac{IRSc}{10^6 \text{ mg/kg}} \right) \times FC} \quad (3-1)$$

**3.1.2 RBC for Residential Soil - Cancer Endpoint.** A residential soil RBC for a cancer endpoint can be estimated using the following formula (USEPA, 1996a):

$$RBC_s = \frac{TR \times ATc}{Efr \times \left( \frac{IFSadj}{10^6 \text{ mg/kg}} \right) \times FC \times CPSo} \quad (3-2)$$

**3.1.3 RBC for Industrial Soil - Noncancer Endpoint.** An industrial soil RBC for a noncancer endpoint can be estimated using the following formula (USEPA, 1996a):

$$RBC_{is} = \frac{THQ \times RfDo \times BWa \times ATn}{EFi \times EDi \times \left( \frac{IRSa}{10^6 \text{ mg/kg}} \right) \times FC} \quad (3-3)$$

**3.1.4 RBC for Industrial Soil - Cancer Endpoint.** An industrial soil RBC for a cancer endpoint can be estimated using the following formula (USEPA, 1996a):

$$RBC_{is} = \frac{TR \times BWa \times ATc}{EFi \times EDi \times \left( \frac{IRSa}{10^6 \text{ mg/kg}} \right) \times FC \times CPSo} \quad (3-4)$$

Table 3-1. Parameters used in Risk-Based Concentration (RBC) equations		
Abbrev.	Definition	Value
RBCrs	Risk-Based Concentration for residential soil	mg chemical/kg soil
RBCis	Risk-Based Concentration for industrial soil	mg chemical/kg soil
THQ	Toxicity Hazard Quotient	1
TR	Target Cancer Risk	10 <sup>-5</sup> (residential) 10 <sup>-4</sup> (industrial)
RfDo	Oral Reference Dose	mg chemical/kg body weight/day (Table 1-2)
RfDi	Inhalation Reference Dose	mg chemical/kg body weight/day (Table 1-2)
CPSi	Cancer slope factor, inhalation	(mg/kg/day) <sup>-1</sup> (Table 1-2)
CPSo	Cancer slope factor, oral	(mg/kg/day) <sup>-1</sup> (Table 1-2)
BWa	Body weight, adult	70 kg
BWc	Body weight, child	15 kg
ATn	Averaging time for noncancer effects	ED x 365 days
ATc	Averaging time for cancer effects	70 yr x 365 days/yr
K	Volatilization constant for water	0.5 L/m <sup>3</sup>
IRAA	Inhalation rate, adult	20 m <sup>3</sup> /day
IFAadj	Inhalation factor, age-adjusted	11.66 m <sup>3</sup> ·yr/kg·days
IFSadj	Soil ingestion factor, age-adjusted	114.29 mg·yr/kg·days
IRSc	Soil ingestion rate, child	200 mg/day
IRSa	Soil ingestion rate, adult	100 mg/day

FC	Fraction ingested from contaminated source	100% for residential 50% for industrial
EDr	Exposure duration, residential	30 yr
EDc	Exposure duration, child	6 yr
EDi	Exposure duration industrial	25 yr
EFr	Exposure frequency, residential	350 days/yr
EFi	Exposure frequency, industrial	250 days/yr

SOURCE: derived from USEPA 1996a, with modifications

### 3.2 PRELIMINARY REMEDIATION GOALS (PRGs)

Preliminary remediation goals were originally developed as part of the Risk Assessment Guidance for Superfund (USEPA, 1991a). The PRG method has been adopted by USEPA Region IX (USEPA, 1996b). Region IX models are currently used establish PRGs for exposure to residential tapwater, residential and industrial soil, and ambient air. For the chemical warfare agents discussed in this report PRG models are used to calculate screening levels only for residential and industrial soil. The parameters used in the PRG equations are listed in Table 3-2. The abbreviations for these parameters are those used by USEPA Region IX (USEPA, 1996b).

**3.2.1 PRG for Residential Soil - Noncancer Endpoint.** A PRG for volatile or semivolatile chemical contaminants in residential soil can be estimated using the following USEPA Region IX equation (USEPA, 1996b):

$$PRG_{rs} = \frac{THQ \times BW_c \times AT_n}{EF_r \times ED_c \times \left( \left( \frac{1}{RfD_o} \times \frac{IRS_c}{10^6 \text{ mg/kg}} \right) + \left( \frac{1}{RfD_o} \times \frac{SA_c \times AF \times ABS}{10^6 \text{ mg/kg}} \right) + \left( \frac{1}{RfD_i} \times \frac{IRA_c}{VF_s} \right) \right)} \quad (3-5)$$

**3.2.4 PRG for Residential Soil - Cancer Endpoint.** The cancer-based PRG for residential soil can be estimated from the following USEPA Region IX equation (USEPA, 1996b):

$$PRG_{rs} = \frac{TR \times AT_c}{EF_r \times \left( \left( \frac{IFS_{adj} \times CSF_o}{10^6 \text{ mg/kg}} \right) + \left( \frac{SFS_{adj} \times ABS \times CSF_o}{10^6 \text{ mg/kg}} \right) + \left( \frac{InhF_{adj} \times CSF_i}{VF_s} \right) \right)} \quad (3-6)$$

**3.2.5 PRG for Industrial Soil - Noncancer Endpoint.** A PRG for a noncancer endpoint for volatile or semivolatile chemical contaminants in industrial soil can be estimated using the following USEPA Region IX equation (USEPA, 1996b):

$$PRG_{is} = \frac{THQ \times BW_a \times AT_n}{EF_i \times ED_i \times \left( \left( \frac{1}{RfD_o} \times \frac{IRS_i}{10^6 \text{ mg/kg}} \right) + \left( \frac{1}{RfD_o} \times \frac{SA_a \times AF \times ABS}{10^6 \text{ mg/kg}} \right) + \left( \frac{1}{RfD_i} \times \frac{IRA_a}{VF_s} \right) \right)} \quad (3-7)$$

**3.2.6 PRG for Industrial Soil - Cancer Endpoint.** A PRG for a cancer endpoint for volatile or semivolatile chemical contaminants in industrial soil can be estimated using the following USEPA Region IX equation (USEPA, 1996b):

$$PRG_{is} = \frac{TR \times BW_a \times AT_c}{EF_i \times ED_i \times \left( \left( \frac{IRS_i \times CSF_o}{10^6 \text{ mg/kg}} \right) + \left( \frac{SA_a \times AF \times ABS \times CSF_o}{10^6 \text{ mg/kg}} \right) + \left( \frac{IRA_a \times CSF_i}{VF_s} \right) \right)} \quad (3-8)$$

**Note:** In Equations 3-7 and 3-8, the soil ingestion rate (SA<sub>a</sub>) of 50 mg/day incorporates the fraction of soil ingested from the contaminated site (50%), and the inhalation rate (IRA<sub>a</sub>) of 10 m<sup>3</sup>/day is for an 8-hour work day; therefore, an adjustment for fraction of the day at the site is not needed.

Table 3-2. Parameters used in equations for Preliminary Remediation Goals (PRGs)		
Abbrev.	Definition	Value
PRG <sub>rs</sub>	Preliminary Remediation Goal for residential soil	mg chemical/kg soil
PRG <sub>is</sub>	Preliminary Remediation Goal for industrial soil	mg chemical/kg soil
THQ	Toxicity Hazard Quotient	1
TR	Target Cancer Risk	10 <sup>-5</sup> (residential) 10 <sup>-4</sup> (industrial)
RfD <sub>o</sub>	Oral Reference Dose	mg chemical/kg body weight/day (Table 1-2)
RfD <sub>i</sub>	Inhalation Reference Dose	mg chemical/kg body weight/day (Table 1-2)
CSF <sub>i</sub>	Cancer slope factor, inhalation	(mg/kg/day) <sup>-1</sup> (Table 1-2)
CSF <sub>o</sub>	Cancer slope factor, oral	(mg/kg/day) <sup>-1</sup> (Table 1-2)
BW <sub>a</sub>	Body weight, adult	70 kg
BW <sub>c</sub>	Body weight, child	15 kg
AT <sub>n</sub>	Averaging time for noncancer effects	ED x 365 days
AT <sub>c</sub>	Averaging time for cancer effects	70 yr x 365 days/yr
IRA <sub>a</sub>	Inhalation rate, adult	20 m <sup>3</sup> /day

$IRA_c$	Inhalation rate, child	10 m <sup>3</sup> /day
$InF_{adj}$	Inhalation factor, age-adjusted	11 (m <sup>3</sup> ·yr/kg·days)
$IFS_{adj}$	Soil ingestion factor, age-adjusted	114 mg·yr/kg·day
$SFS_{adj}$	Skin contact factor, age-adjusted	504 mg·yr/kg·days
$IRS_c$	Soil ingestion rate, child	200 mg/day
$IRS_a$	Soil ingestion rate, adult	100 mg/day
$IRS_i$	Soil ingestion rate, industrial	50 mg/day
$SA_a$	Exposed body surface area, adult	5700 cm <sup>2</sup>
$SA_c$	Exposed body surface area, child	2900 cm <sup>2</sup>
$VF_s$	Volatilization factor for soil	chemical specific (Table 2-3)
PEF	Particulate emission factor	1.32 x 10 <sup>9</sup> m <sup>3</sup> /kg
ABS	Dermal absorption factor, chemical specific (see Table 2-4)	12 hr cumulative, residential 8 hr cumulative, industrial
$AF_a$	Soil-to-skin adherence factor, adult	0.08 mg/cm <sup>2</sup>
$AF_c$	Soil-to-skin adherence factor, child	0.3 mg/cm <sup>2</sup>
$ED_{tot}$	Exposure duration, total	30 yr
$ED_r$	Exposure duration, residential	30 yr
$ED_c$	Exposure duration, child	6 yr
$ED_i$	Exposure duration, industrial	25 yr
$EF_r$	Exposure frequency, residential	350 days/yr
$EF_i$	Exposure frequency, industrial	250 days/yr

SOURCE: Derived from USEPA 1996b, with modifications

### 3.3 SOIL SCREENING LEVELS (SSLs)

Soil screening levels are derived only for residential exposure scenarios (USEPA, 1996c). SSLs for surface soils include separate calculations for direct ingestion of soil particles and inhalation of fugitive dust particles. Exposure through dermal contact with contaminated surface soils is also considered a possible exposure pathway; however, incorporation of the dermal pathway is considered to be limited by the available quantitative data on dermal absorption rates for specific chemicals. USEPA (1996c) notes that if the estimated dermal absorption of a chemical is greater than 10%, as in the case of pentachlorophenol, the ingestion SSL should be divided in half to account for the assumption that exposure via the dermal route is equivalent to the ingestion route.

SSLs for subsurface soils address two exposure pathways: ingestion of ground water contaminated as a result of the migration of the chemicals through the soil to the underlying aquifer, and inhalation of volatile compounds released from soil. Groundwater is not considered a probable concern at most sites (see discussion in Section 1.3.3 and Appendix E). Site specific information is necessary to assess screening levels based on concerns about the potential of agent being a source of risk from groundwater contamination. Therefore this pathway is not included in the following calculations. The parameters used in the SSL equations are listed in Table 3-3. The abbreviations of the parameters (without the subscripts) are those used by OSWER (USEPA, 1996c).

The overall SSL methodology involves assessing each pathway separately and selecting the most conservative value (most sensitive exposure pathway) as a screening level. The pathway however should be consistent with realistic site conditions (i.e. the pathway should be considered a completed pathway of exposure).

**3.3.1 SSL for Ingestion of Contaminants in Residential Soil - Noncancer Endpoint.** The equation for deriving an SSL based on noncancer effects for ingestion of contaminated residential soil is as follows (USEPA, 1996c):

$$SSL = \frac{THQ \times BW_c \times AT_n \times 365 \text{ days/yr}}{1/RfD_o \times 10^{-6} \text{ kg/mg} \times EF_r \times ED_c \times IR_c} \quad (3-9)$$

**3.3.2 SSL for Ingestion of Contaminants in Residential Soil - Cancer Endpoint.** The equation for deriving an SSL based on cancer effects for ingestion of contaminated residential soil is as follows (USEPA, 1996c):

$$SSL = \frac{TR \times AT_c \times 365 \text{ days/yr}}{SF_o \times 10^{-6} \text{ kg/mg} \times EF_r \times IF_{soil/adj}} \quad (3-10)$$

**3.3.3 SSL for Inhalation of Fugitive Dust in Residential Soil - Noncancer Endpoint.** The equation for deriving an SSL based on noncancer effects for inhalation of fugitive dusts from residential surface soil is as follows (USEPA, 1996c):

$$SSL = \frac{THQ \times AT_n \times 365 \text{ days/yr}}{EF_r \times ED_r \times \left(\frac{1}{RfC} \times \frac{1}{PEF}\right)} \quad (3-11)$$

**3.3.4 SSL for Inhalation of Fugitive Dust in Residential Soil - Cancer Endpoint.** The equation for deriving an SSL based on cancer effects for inhalation of fugitive dusts from residential surface soil is as follows (USEPA, 1996c):

$$SSL = \frac{TR \times AT_c \times 365 \text{ days/yr}}{URF \times 1,000 \text{ } \mu\text{g/mg} \times EF_r \times ED_r \times \left(\frac{1}{PEF}\right)} \quad (3-12)$$

**3.3.5 SSL for Inhalation of Volatile Organics in Residential Soil - Noncancer Endpoint.** The equation for deriving an SSL based on noncancer effects for inhalation of volatile organics released from residential subsurface soil is as follows (USEPA, 1996c):

$$SSL_v = \frac{THQ \times AT_n \times 365 \text{ days/yr}}{EF_r \times ED_r \times \left(\frac{1}{RfC} \times \frac{1}{VF}\right)} \quad (3-13)$$

The volatilization factor (VF) is derived from Equation A-24 in Appendix A. Because the equation to calculate an SSL for inhalation of volatiles from contaminated soils assumes an infinite source, it can violate mass-balance considerations, especially for small sources. The Soil Screening Guidance, therefore, also includes a method for calculating mass-limit SSLs when the size (i.e., area and depth) of the contaminated soil source is known or can be estimated with confidence. The mass-limit VF is derived from the following equation (USEPA, 1996c):

$$VF = Q/C \times \frac{[T \times (3.15 \times 10^7 \text{ s/yr})]}{(\rho_b \times d_s \times 10^6 \text{ g/Mg})} \quad (3-14)$$



where:

VF	=	Volatilization factor
Q/C	=	Inverse of mean concentration at center of a square source (USEPA default = 68.81 g/m <sup>2</sup> -s per kg/m <sup>3</sup> )
T	=	Exposure interval (USEPA default = 9.5 x 10 <sup>8</sup> s)
ρ <sub>b</sub>	=	Dry soil bulk density (USEPA default = 1.5 kg/L or Mg/m <sup>3</sup> )
d <sub>s</sub>	=	Average source depth in m (site-specific)

**3.3.6 SSL for Inhalation of Volatile Organics in Residential Soil - Cancer Endpoint.** The equation for deriving an SSL based on cancer effects for inhalation of volatile organics released from residential subsurface soil is as follows (USEPA, 1996c):

$$SSL_v = \frac{TR \times AT_n \times 365 \text{ days/yr}}{URF \times 1,000 \text{ } \mu\text{g/mg} \times EF_r \times ED_r \times \left(\frac{1}{VF}\right)} \quad (3-15)$$

The VF is derived from Equation 2-1. Because the equation to calculate a SSL for inhalation of volatiles from contaminated soils assumes an infinite source, it can violate mass-balance considerations, especially for small sources. The Soil Screening Guidance, therefore, also includes a method for calculating mass-limit SSLs when the size (i.e., area and depth) of the contaminated soil source is known or can be estimated with confidence (see Section 3.3.5).

### 3.3.7 SSL for Migration of Contaminants to Ground Water

As stated by USEPA (1996c), the simplifying assumptions used in deriving SSLs based on migration of contaminants to ground water include the following:

- Infinite source (steady-state concentrations maintained over the exposure period).
- Uniformly distributed contamination from the surface to the top of the aquifer.
- No contaminant attenuation (i.e., adsorption, biodegradation, chemical degradation) in soil.
- Instantaneous and linear equilibrium soil/water partitioning.
- Unconfined, unconsolidated aquifer with homogeneous and isotropic hydrologic properties.
- Receptor well at the downgradient edge of the source and screened within plume.
- No contaminant attenuation in the aquifer.
- Contaminant not present as nonaqueous phase liquid (NAPL). If NAPL is present, then the SSL does not apply.

The equation used to derive an SSL based on migration of the chemical contaminant to ground water is as follows (USEPA, 1996c):

$$SSL = C_w \left[ K_d + \frac{(\Theta_w + \Theta_a H')}{\rho_b} \right] \quad (3-16)$$

where:

- $C_w$  = Target soil leachate concentration; nonzero MCLG, MCL, or HBL x DAF (in mg/L)
- $K_d$  = Soil-water partition coefficient in L/kg (chemical-specific =  $K_{oc} \times f_{oc}$ )
- $K_{oc}$  = Soil organic carbon-water partition coefficient in L/kg (chemical -specific)
- $f_{oc}$  = Fraction organic carbon in soil (0.002)
- $\Theta_w$  = Water-filled soil porosity ( $0.3 L_{water}/L_{soil}$ )
- $\Theta_a$  = Air-filled soil porosity ( $n - \Theta_w$ )
- $n$  = Soil porosity in  $L_{pore}/L_{soil}$  [ $1 - (\rho_b/\rho_s)$ ]
- $\rho_b$  = Dry soil bulk density (1.5 kg/L)
- $\rho_s$  = Soil particle density (2.65 kg/L)
- $H'$  = Dimensionless Henry's Law Constant (chemical-specific)

The use of the above equation to calculate an SSL assumes an infinite source of contaminants extending to the top of the aquifer. Contaminants at sites with shallow sources, thick unsaturated zones, degradable contaminants, or unsaturated zone characteristics (e.g., clay layers) may attenuate before they reach ground water. In such cases unsaturated zone models and a mass-limit SSL should be calculated when the area and depth (i.e., volume) of the source are known or can be estimated reliably (see Section 3.3.7.3) (USEPA, 1996d).

### 3.3.7.1 Health-Based Limits (HBLs)

If a drinking water standard (e.g. Maximum Contaminant Level) is not available to determine the target soil leachate concentration, the  $C_w$  can be derived from an HBL which is the oral RfD for the chemical multiplied by the average body weight of 70 kg and divided by the daily water consumption rate of 2 L. Thus, the HBL for a chemical with an oral RfD of 1 mg/kg/day would be 35 mg/L, and the target soil leachate concentration would be 700 mg/L (using a 20-fold dilution factor). For a carcinogen, the HBL can be fixed at the drinking water concentration corresponding to a specific risk level.

### 3.3.7.2 Derivation of the Dilution Factor

As soil leachate moves through the soil and ground water, contaminant concentrations are attenuated by adsorption and degradation (USEPA, 1996c). In the aquifer, dilution by ground water further reduces contaminant concentrations. This reduction in concentration can be expressed by a dilution attenuation factor (DAF), defined as the ratio of soil leachate concentration to receptor point concentration. USEPA's Soil Screening Guidance addresses only one attenuation process -- contaminant dilution in ground water. Furthermore, because of the uncertainty resulting from the wide variability in subsurface conditions, a default DAF of 20 has been selected as protective for contaminated soil sources up to 0.5 acres in size. Thus, if the

health-based limit for ground water is 1 mg/L, then the target soil leachate concentration is 20 mg/L. A DAF of 20 has been used in the calculations of the SSLs for the chemical warfare agents. USEPA notes that because SSLs based on migration to ground water are very sensitive to DAF, site-specific dilution factors should be calculated whenever possible.

### 3.3.7.3 Mass-Limit SSL for Migration to Ground Water

Because the SSL for ground water assumes an infinite source, it can violate mass-balance considerations, especially for small sources. The Soil Screening Guidance, therefore, also includes a method for calculating mass-limit SSLs when the size (i.e., area and depth) of the contaminated soil source is known or can be estimated with confidence. The mass-limit SSL can be estimated using the following equation (USEPA, 1996c):

$$SSL_{gw} = \frac{(C_w \times l \times ED)}{\rho_b \times d_s} \quad (3-17)$$

where:

- SSL = Soil Screening Level (mg/kg)  
 CW = Target soil leachate concentration in mg/L (nonzero MCLG, MCL, or HBL x dilution factor)  
 l = Infiltration rate (0.18 m/yr)  
 ED = Exposure duration (70 yr)  
 $\rho_b$  = Dry soil bulk density (1.5 kg/L)  
 $d_s$  = Depth of source in m (site-specific)

Table 3-3. Parameters used in equations for Soil Screening Levels (SSLs)		
Abbrev.	Definition	Value
SSL	Soil Screening Level	mg chemical/kg soil
THQ	Toxicity Hazard Quotient	1
TR	Target Cancer Risk	$10^{-5}$ , residential
RfD <sub>o</sub>	Oral Reference Dose	mg/kg/day (Table 1-2)
RfC	Inhalation Reference Concentration	mg/m <sup>3</sup> (Table 1-2)
URF	Inhalation unit risk factor	( $\mu\text{g}/\text{m}^3$ ) <sup>-1</sup>
CPS <sub>o</sub>	Cancer slope factor, oral	(mg/kg/day) <sup>-1</sup> (Table 1-2)
BW <sub>c</sub>	Body weight, child	15 kg

AT <sub>n</sub>	Averaging time for noncancer effects	6 yr, child 30 yr, adult
AT <sub>c</sub>	Averaging time for cancer effects	70 yr
IR <sub>c</sub>	Soil ingestion rate, child	200 mg/day
IF <sub>soil/adj</sub>	Soil ingestion rate, age-adjusted	114 mg·yr/kg·day
ED <sub>r</sub>	Exposure duration, residential	30 yr
ED <sub>c</sub>	Exposure duration, child	6 yr
EF <sub>r</sub>	Exposure frequency, residential	350 days/yr
PEF	Particulate Emission Factor	1.32 x 10 <sup>9</sup> m <sup>3</sup> /kg
SOURCE: Derived from USEPA 1996c, with modifications		

#### 4. AGENT HD

HBESLS for agent HD, as derived from the algorithms presented in Section 3, are summarized in Table 4-1. The toxicity values and chemical-specific parameter values used to calculate the HBESLS are listed in Table 4-2. As HD is a known carcinogen, both cancer and noncancer endpoints are evaluated.

For noncancer endpoints an oral RfD of 0.000007 mg/kg/day is used. The inhalation RfD is derived from the DHHS/Army air control limit of 0.0001 mg/m<sup>3</sup> by assuming an inhalation rate of 20 m<sup>3</sup>/day and a body weight of 70 kg. The resulting inhalation RfD is 0.00003 mg/kg/day. The exposure parameters used to calculate the RBCs, PRGs and SSLs are described in detail in Sections 2 and 3.

Table 4-1. Summary of calculated HBESLS for agent HD				
Method (units)	Media, Scenario (pathways)	Noncancer Derived Value	Cancer <sup>a</sup> Derived Value	HBESL
<b>Region III</b>				
RBC (mg/kg)	Soil, residential (ingestion)	0.55	0.83 <sup>b</sup>	0.55
RBC (mg/kg)	Soil, commercial/industrial (ingestion)	14	74 <sup>c</sup>	14
<b>Region IX</b>				
PRG (mg/kg)	Soil, residential (ingestion, vapor inhalation, dermal)	0.4	0.01 <sup>b</sup>	0.01 <sup>b</sup>
PRG (mg/kg)	Soil, commercial/industrial (ingestion, vapor inhalation, dermal)	4.5	0.3 <sup>c</sup>	0.3 <sup>c</sup>
<b>OSWER</b>				
SSL (mg/kg)	Soil, residential (ingestion)	0.55	0.83 <sup>b</sup>	
SSL (mg/kg)	Soil, residential (inhalation of dusts)	1.4 x 10 <sup>5</sup>	378 <sup>b</sup>	
SSL (mg/kg)	Soil, residential (inhalation of volatiles)	5.9	0.016 <sup>b</sup>	0.016 <sup>b</sup>
SSL (mg/kg)	Soil, residential (migration to ground water)	site-specific <sup>d</sup>	site-specific <sup>d</sup>	

<sup>a</sup> Oral slope factor of 7.7 (mg/kg/day)<sup>-1</sup> (see Section 1.2.4)

<sup>b</sup> Target cancer risk level of 10<sup>-5</sup>

<sup>c</sup> Target cancer risk level of 10<sup>-4</sup>

<sup>d</sup> Because the potential for migration to ground water is quite low, it is recommended that a site-specific analysis of this HBESL be conducted only for those situations where ground-water contamination water is a concern

Table 4-2. Toxicity values and environmental parameters for agent HD		
Parameter	Value	Units
Oral Reference Dose	0.000007	mg/kg/day
Air exposure limit	0.0001	mg/m <sup>3</sup>
Inhalation Reference Dose	0.00003	mg/kg/day
Oral slope factor	7.7	(mg/kg/day) <sup>-1</sup>
Inhalation unit risk	0.085	(µg/m <sup>3</sup> ) <sup>-1</sup>
Inhalation slope factor	300	(mg/kg/day) <sup>-1</sup>
Dermal absorption factor <sup>d</sup>	5.6/12 hr (residential) 8.4/8 hr (industrial)	percent, from soil
Vapor pressure <sup>a</sup>	0.11	mm Hg at 25 °C
Solubility <sup>a</sup>	0.92	g/L at 22 °C
Henry's Law Constant (H) <sup>b</sup>	2.1 x 10 <sup>-5</sup>	atm m <sup>3</sup> /mol
Volatilization factor (VF) <sup>b</sup>	5.62 x 10 <sup>4</sup>	m <sup>3</sup> /kg
Soil-water partition coefficient (K <sub>d</sub> ) <sup>c</sup>	0.266	unitless
Hydrolysis half-life <sup>c</sup>	0.083	hr at 22 °C (acidic)
Persistence in soil	0.038 <sup>c</sup> - <1.0 <sup>a</sup> 1+ <sup>a</sup> - 3 <sup>c</sup>	yr, on soil surface yr, buried in soil

<sup>a</sup> Value from Rosenblatt et al., 1995

<sup>b</sup> see Appendix A

<sup>c</sup>  $K_d = K_{oc} \times f_{oc}$ ;  $f_{oc} = 0.006$  g organic carbon/g soil (OSWER default);  $K_{oc}$  = soil organic carbon-water partition coefficient ( $\log K_{oc} = 1.377 + 0.544 \log K_{ow}$ ; where  $K_{ow}$  = water-octanol partition coefficient)

<sup>d</sup> See Section 2.3.2.2 and Appendix H

<sup>e</sup> Value from DA, 1974

The derivation of cancer-based HBESLS for agent HD is complicated by several uncertainties associated with the quantification of the carcinogenic potency of the agent (see discussion in Section 1.2.4). Oral slope factors ranging from 1.6 to 95 (mg/kg/day)<sup>-1</sup> have been derived for HD. In developing HBESLS in this report, the geometric mean value of 7.7 (mg/kg/day)<sup>-1</sup> is used. An inhalation slope factor of 300 (mg/kg/day)<sup>-1</sup> was estimated from the inhalation unit risk recommended by USEPA (1991b) and identified as an interim value by OTSG (DA, 1996a). The target cancer risk level is a risk management decision that

should be made on a site-specific basis. However, a single value is needed to calculate predetermined HBESLS. In this document, a target cancer risk level of  $10^{-5}$  is used to calculate residential HBESLS and a target cancer risk level of  $10^{-4}$  is used to calculate industrial/commercial HBESLS. The rationale for using these risk levels is discussed in Section 1.3.2.

#### 4.1 RISK-BASED CONCENTRATIONS (RBCs)

The soil RBCs for HD are based on a single exposure pathway, incidental ingestion of contaminated soil. The maximum RBC is 74 mg/kg soil for commercial/industrial exposure scenario. At this HBESL, the HD dose resulting from the incidental ingestion of 50 mg of soil (the USEPA default for soil ingestion) is approximately 0.003 mg. In comparison, in studies conducted on rats, a dose of 0.03 mg/kg (about 0.01 mg/animal) caused no toxic effects or produced only mild signs of toxicity after repeated exposures for 13 weeks (see Section 1.3.8). This comparison is based on the assumption that the agent is evenly dispersed through the soil; however, it should be emphasized that if the agent is concentrated into discrete masses in the soil, there is a much greater potential for acute toxicity since a dose of only 0.8 mg is known to cause severe damage to the gastric mucosa in experimental animals.

Although RBCs do not directly address dermal exposures, the potential for acute dermal toxicity at the maximum RBC can be estimated. Assuming an exposed skin area of 5700 cm<sup>2</sup> for adults, and a soil-to-skin adherence of 0.08 mg per cm<sup>2</sup> of skin, the amount of soil that may be in contact with the skin is 456 mg and, at the HBESL of 74 mg/kg, this quantity of soil would contain about 0.03 mg of HD (34 µg). If evenly dispersed in the soil, the average amount of HD per square centimeter of exposed skin would be 0.006 µg (34 µg/5700 cm<sup>2</sup>). In comparison, amounts as small as 2 µg are likely to cause erythema in many exposed individuals and blistering in some (see Section 1.3.8). As noted above, if the HD is concentrated into discrete masses in the soil, then there is a significantly increased potential for acute toxicity. Obviously, the RBC methodology (which models chronic health risks) would not apply in such cases where acute toxicity is a realistic concern..

#### 4.2 PRELIMINARY REMEDIATION GOALS (PRGs)

The residential and industrial soil PRGs are substantially less than the corresponding soil RBCs; therefore, the potential for acute exposures is considerably reduced.

For PRGs, volatilization of HD is considered a potential exposure pathway; therefore, the VF of  $5.62 \times 10^4$  m<sup>3</sup>/kg is used in the calculations. Because of the relatively large inhalation unit risk, the oral and dermal exposure pathways contribute relatively little to final cancer PRGs. For example, a cancer-based residential soil PRG derived only from the combined oral and dermal pathways is about 0.6 mg/kg, but one based on only the inhalation pathway is 0.01 mg/kg.

The maximum PRGs are 0.4 mg/kg for residential and 4.5 mg/kg for industrial scenarios. At 4.5 mg/kg, the HD air concentration could theoretically equal  $0.00008 \text{ mg/m}^3$ , assuming that the air concentration is a function of the soil concentration (4.5 mg/kg) divided by the VF ( $5.62 \times 10^4 \text{ m}^3/\text{kg}$ ). Rosenblatt et al. (1995) calculated that for an initial HD soil concentration of 1.0 mg/kg (at a depth of 2-3 m and covering  $10,000 \text{ m}^2$ ), the theoretical average air exposure concentration downwind (windspeed 10 mph) over 90 days would be  $0.0085 \text{ } \mu\text{g/m}^3$  ( $0.0000085 \text{ mg/m}^3$ ). Rosenblatt et al. (1995) noted that empirical evidence and measured reactivity of HD with water suggest that this is a very conservative estimate. In comparison, a CT of  $12 \text{ mg-min/m}^3$  ( $0.2 \text{ mg/m}^3$  for 60 min) has been reported to be a no-effect level for eye irritation (see Section 1.3.8). The maximum allowable CT for skin effects is  $5 \text{ mg-min/m}^3$  and for eye effects it is  $2 \text{ mg-min/m}^3$  (DA, 1974); these values equate to 0.083 and  $0.033 \text{ mg/m}^3$  for 60-min exposures, respectively.

### 4.3 SOIL SCREENING LEVELS (SSLs)

The cancer-based SSLs are lower than the noncancer SSLs. For deriving an SSL for inhalation of fugitive dusts in residential soil, the USEPA default PEF of  $1.32 \times 10^9 \text{ m}^3/\text{kg}$  is applied. It should be noted that this HBESL is presented here only to show the results of the calculation following USEPA's guidelines, and is by no means a recommendation for use in remediation. USEPA states that the SSL for inhalation of fugitive dust does not need to be routinely calculated for organic compounds because it is usually several orders of magnitude higher than the corresponding generic ingestion SSLs. For derivation of an SSL for inhalation of volatiles released from soils, the VF<sub>s</sub> of  $5.62 \times 10^4 \text{ m}^3/\text{kg}$  is used. This resulted in a cancer SSL of  $0.016 \text{ mg/kg}$ , very similar to the residential soil PRG of  $0.01 \text{ mg/kg}$ , indicating again that the inhalation pathway is a primary factor for determining the soil screening level.

An SSL for migration to ground water was not calculated for agent HD. The methodology for this SSL assumes an infinite source and no degradation, conditions which are not likely to apply to HD. The actual potential for agent HD migration to ground water is considered to be quite low (see Appendix E). For this reason, it is recommended that a site-specific analysis be conducted for those situations where ground-water contamination is a concern.

Although HD may remain in the soil for months to years, this material is usually present in the form of encapsulated globules, the coating of which prevents further dissolution and degradation (Rosenblatt et al., 1995). In such cases if the capsules are broken, the potential for an acute hazard is high. HBESLS should not be applied to such situations, but rather only to the residual contamination following removal and disposal of the larger masses of agent.



#### 4.4 SUMMARY

Because it incorporates multipathway exposures, the PRG methodology yields the most conservative HBESLS, and for the selected target cancer levels, the cancer-based PRG model yields levels that are more conservative than the noncancer PRGs. However, as noted in Section 1.3.7, when toxic effects of a chemical are not expected to be additive across pathways, PRGs may be overly conservative. To some degree, this may be the case for vesicants such as HD. Oral exposures to HD are likely to affect primarily the lining of the gastro-intestinal tract; dermal exposures target the skin; and inhalation exposures may damage the respiratory tract (and possibly also affect the eyes and skin). RBCs for HD may therefore be adequately protective. However, site-specific evaluation of potential inhalation and dermal pathways (including potential for acute effect levels) may need to be evaluated. SSLs are very similar to the residential PRGs, due to the impacts of including the inhalation pathway.

## 5. AGENT VX

The HBESLs for VX, as derived from the algorithms presented in Section 3, are summarized in Table 5-1. The toxicity values and the environmental parameter values used to calculate the HBESLs are listed in Table 5-2. The exposure parameters used to calculate the RBCs, PRGs, and SSLs are described in detail in Sections 2 and 3. The oral RfD for VX is  $6 \times 10^{-7}$  mg/kg/day. The estimated inhalation RfD for VX of  $9 \times 10^{-8}$  mg/kg/day was derived from recent suggested revisions to the DHHS/Army control limit (currently 0.000003 mg/m<sup>3</sup>, suggested modification is an order of magnitude lower at 0.0000003 mg/m<sup>3</sup>) by assuming an inhalation rate of 20 m<sup>3</sup>/day and a default body weight of 70 kg. Because there is no evidence that VX is carcinogenic, HBESLs were calculated only for noncarcinogenic effects.

Table 5-1. Summary of calculated HBESLs for agent VX			
Method (units)	Media, Scenario (pathways)	Derived Value	HBESL
			Noncancer Only
Region III			
RBC (mg/kg)	Soil, residential (ingestion)		0.047
RBC (mg/kg)	Soil, commercial/industrial (ingestion)		1.2
Region IX			
PRG (mg/kg)	Soil, residential (ingestion, dust inhalation, and dermal)		0.042
PRG (mg/kg)	Soil, commercial/industrial (ingestion, dust inhalation, and dermal)		1.1
OSWER			
SSL (mg/kg)	Soil, residential (ingestion)	0.047	0.047
SSL (mg/kg)	Soil, residential (inhalation of dusts)	410	
SSL (mg/kg)	Soil, residential (inhalation of vapors)	0.3	
SSL (mg/kg)	Soil, residential (migration to ground water)	site-specific <sup>a</sup>	

<sup>a</sup> Because the potential for migration to ground water is quite low, it is recommended that a site-specific analysis of this SSL be conducted only for those situations where ground-water contamination is a concern.

<b>Table 5-2. Toxicity values and environmental parameters for agent VX</b>		
<b>Parameter</b>	<b>Value</b>	<b>Units</b>
Oral Reference Dose	0.0000006	mg/kg/day
Inhalation Exposure Limit	0.000003	mg/m <sup>3</sup>
Inhalation Reference Dose	0.00000009	mg/kg/day
Dermal absorption factor	0.27 <sup>f</sup>	percent per hr from soil
Vapor pressure <sup>a</sup>	0.0007	mm Hg
Water solubility <sup>a</sup>	10-50 <sup>h</sup>	g/L
Henry's Law Constant (H) <sup>b</sup>	3.5 x 10 <sup>-9</sup>	atm m <sup>3</sup> /mol
Volatilization factor (VF <sub>s</sub> ) <sup>c</sup>	9.67 x 10 <sup>5</sup>	m <sup>3</sup> /kg
Soil-water partition coefficient (K <sub>d</sub> ) <sup>d</sup>	1.962	NA
Hydrolysis half-life <sup>a</sup>	50 (pH 9) - 2000 (pH 5)	hr
Persistence in soil	2-6 <sup>g</sup> <90 <sup>e</sup>	days

<sup>a</sup> Value from MacNaughton and Brewer, 1994

<sup>b</sup> Value from Small, 1984

<sup>c</sup> see Appendix A

<sup>d</sup>  $K_d = K_{oc} \times f_{oc}$ ;  $f_{oc} = 0.006$  g organic carbon/g soil (OSWER default);  $K_{oc}$  = soil organic carbon-water partition coefficient ( $\log K_{oc} = 1.377 + 0.544 \log K_{ow}$ ; where  $K_{ow}$  = water-octanol partition coefficient)

<sup>e</sup> Value from Rosenblatt et al., 1995, for worst-plausible conditions

<sup>f</sup> see Section 2.3.2.2 and Appendix H

<sup>g</sup> Value from DA, 1974

<sup>h</sup> Value of 30g/L used in calculations

## 5.1 RISK-BASED CONCENTRATIONS (RBCs)

The equations for calculating USEPA Region III RBCs (USEPA, 1996a) are given in Section 3.1. The soil RBC is based solely on incidental ingestion of contaminated soil. The industrial soil RBC is 1.2 mg/kg, and the dose resulting from the incidental ingestion of 50 mg of soil would be approximately 0.00006 mg VX. In tests on humans, an oral dose of about 0.1 mg (calculated from a reported dose of 0.0014 mg/kg/day and a default body weight of 70 kg) caused no signs of toxicity even after 7 days of exposure (see Section 1.3.8).

## 5.2 PRELIMINARY REMEDIATION GOALS (PRGs).

The USEPA Region IX equations for PRGs are given in Section 3.2. The dermal absorption factor used in the calculation of the residential soil PRGs is 3.24% for a 12-hour period. The dermal absorption value used for the industrial soil PRG is 2.2% for an 8-hour period. The inhalation pathway is not included in the soil PRG because VX is not expected to volatilize from soil (Henry's Law Constant less than  $1 \times 10^{-5}$  atm-m<sup>3</sup>/mol). Instead, the  $VF_s$  in the soil PRG equations is replaced with the particulate emission factor (PEF =  $1.32 \times 10^9$  m<sup>3</sup>/kg) to account for exposure through fugitive dust emissions. Assuming an exposed skin area of 5700 cm<sup>2</sup> for adults, and a soil-to-skin adherence of 0.08 mg per cm<sup>2</sup> of skin, the amount of soil that may be in contact with the skin is 456 mg and, at the HBESL of 1.1 mg/kg, this quantity of soil would contain about 0.5 µg of VX. In comparison, mild signs of toxicity were reported in individuals receiving a percutaneous dose of 320 µg (see Section 1.3.8).

## 5.3 SOIL SCREENING LEVELS (SSLs)

The equations for calculating USEPA OSWER SSLs (USEPA, 1996a) are given in Section 3.3. The residential soil SSL is identical to the residential soil RBC. For deriving an SSL for inhalation of fugitive dusts in a residential soil, the USEPA default PEF of  $1.32 \times 10^9$  m<sup>3</sup>/kg was applied and the resulting SSL is 410 mg/kg. This HBESL is presented here only to show the results of the calculation following USEPA's guidelines, and it is not intended as a recommendation for use in remediation. Other SSLs are more protective and must therefore take precedence. An SSL was also calculated for inhalation of vapors released from soil, even though the likelihood of VX volatilizing from soil is presumed very small. The SSL of 0.3 mg/kg for volatiles is more than 1000-fold more protective than the SSL for dusts; however, the residential soil PRG is still smaller yet. Both the SSL for inhalation pathway and the PRG models are driven by the inhalation pathway, though the SSL approach even more conservatively addresses this pathway by inserting a volatilization factor (VF) in where the PRG assumes only a particulate emission factor (PEF). This difference in the models in some cases (as with the G-agents) results in a lower SSL value than PRG value. But due to the particularly low RfD values for VX (oral and inhalation), the ingestion pathway plays a more significant role, and the additive PRG model, therefore, yields the lowest HBESL value.

An SSL for migration to ground water was not calculated for agent VX. The methodology for this SSL assumes an infinite source and no degradation, conditions which are not likely to apply to VX. The actual potential for agent VX migration to ground water is considered to be quite low (see Appendix E). For this reason, it is recommended that a site-specific analysis be conducted for those situations where contamination of ground water is a concern. The primary hydrolysis product of VX, EA-2192 is expected to be more stable in water, and is considered to be as toxic as VX (see Appendix F). It is recommended that the SSL for migration to groundwater be evaluated for this compound.

## 5.4 SUMMARY

Because the RfDs (oral and inhalation) of agent VX are particularly low (one to two orders of magnitude lower than the other nerve agents) the impacts of both the oral and inhalation pathways on the end result are significant, whereas with other nerve agents the inhalation pathway has a greater impact on the resulting HBESL value. Though the PRG methodology yields the most conservative HBESLs because they incorporate multipathway exposures, the differences between the PRGs, RBCs, and SSLs are minimal in the case of VX. All methods appear to yield appropriate, valid screening values which represent concentrations that do not present acute or chronic health risks for the given scenarios. Therefore, because the differences between methodologies are relatively insignificant, the PRG method may be used to address concerns regarding additive toxicity across exposure pathways.

## 6. AGENT GB

The HBESLs for agent GB, as derived from the algorithms given in Section 3, are summarized in Table 6-1. The toxicity values and the environmental parameter values that were used in calculating the HBESLs are listed in Table 6-2. The exposure parameters used to calculate the RBCs, PRGs, and SSLs are described in detail in Sections 2 and 3. The oral RfD for GB is  $2 \times 10^{-5}$  mg/kg/day. The estimated inhalation RfD for GB of  $9 \times 10^{-7}$  mg/kg/day was derived from the DHHS/Army control limit of 0.000003 mg/m<sup>3</sup> by assuming an inhalation rate of 20 m<sup>3</sup>/day and a default body weight of 70 kg. Because there is no evidence that GB is carcinogenic, HBESLs were calculated only for noncarcinogenic effects.

Table 6-1. Summary of calculated HBESLs for agent GB			
Type of HBESL	Media, Scenario (pathways)	derived value	HBESL
			Noncancer Only
Region III			
RBC (mg/kg)	Soil, residential (ingestion)		1.6
RBC (mg/kg)	Soil, commercial/industrial (ingestion)		41
Region IX			
PRG (mg/kg)	Soil, residential (ingestion, inhalation, and dermal)		1.3
PRG (mg/kg)	Soil, commercial/industrial (ingestion, inhalation, and dermal)		32
OSWER			
SSL (mg/kg)	Soil, residential (ingestion)	1.6	
SSL (mg/kg)	Soil, residential (inhalation of dusts)	4100	
SSL (mg/kg)	Soil, residential (inhalation of vapors)	0.53	0.53
SSL (mg/kg)	Soil, residential (migration to ground water)	Site-specific <sup>a</sup>	

<sup>a</sup> Because the potential for migration to ground water is quite low, it is recommended that a site-specific analysis of this SSL be conducted only for those situations where ground-water contamination is a concern

<b>Table 6-2. Toxicity values and environmental parameters for agent GB</b>		
<b>Parameter</b>	<b>Value</b>	<b>Units</b>
Oral Reference Dose	0.00002	mg/kg/day
Inhalation Exposure Limit	0.000003	mg/m <sup>3</sup>
Inhalation Reference Dose	0.0000009	mg/kg/day
Dermal absorption factor	0.35 <sup>g</sup>	percent per hr from soil
Vapor Pressure <sup>e</sup>	2.94	mm Hg
Solubility <sup>e</sup>	miscible	
Henry's Law Constant (H) <sup>b</sup>	5.34 x 10 <sup>-7</sup>	atm·m <sup>3</sup> /mol
Volatilization factor (VF) <sub>s</sub> <sup>c</sup>	1.7 x 10 <sup>5</sup>	m <sup>3</sup> /kg
Soil-water partition coefficient (K <sub>d</sub> ) <sup>d</sup>	0.208	NA
Hydrolysis half-life <sup>e</sup>	0.5 (pH 9) 250 (pH 6.5) 0.5 (pH 5)	hr
Persistence in soil	≤5 <sup>a</sup> <30 <sup>f</sup>	days

<sup>a</sup> Value from DA, 1974

<sup>b</sup> Value from Small, 1984

<sup>c</sup> see Appendix A

<sup>d</sup>  $K_d = K_{oc} \times f_{oc}$ ;  $f_{oc} = 0.006$  g organic carbon/g soil (USEPA default);  $K_{oc}$  = soil organic carbon-water partition coefficient ( $\log K_{oc} = 1.377 + 0.544 \log K_{ow}$ ; where  $K_{ow}$  = water-octanol partition coefficient)

<sup>e</sup> Values from MacNaughton and Brewer, 1994

<sup>f</sup> Value from Rosenblatt et al., 1995, for worst-plausible conditions

<sup>g</sup> See Section 2.3.2.2 and Appendix H

## 6.1 RISK-BASED CONCENTRATIONS (RBCs)

The soil RBC for GB is based solely on ingestion of contaminated soil. The maximum RBC is 41 mg/kg soil for a commercial/industrial scenario. At this HBESL, the dose resulting from ingestion of 50 mg of soil is approximately 0.002 mg GB. In tests on humans, an oral dose of about 0.15 mg (based on a reported dose of 0.002 mg/kg/day and a default body weight of 70 kg) caused mild signs of toxicity (see Section 1.3.8). This dose is about 75 times larger than that calculated from the soil RBC.

## 6.2 PRELIMINARY REMEDIATION GOALS (PRGs).

The equations for calculating USEPA Region IX PRGs (USEPA, 1996b) are given in Section 3.2. Because GB is not expected to volatilize from soil (Henry's Law Constant =  $5.34 \times 10^{-7}$  atm·m<sup>3</sup>/mol), the VF<sub>s</sub> in the PRG equation is replaced with the particulate emission factor (PEF =  $1.32 \times 10^9$  m<sup>3</sup>/kg) to account for exposure through fugitive dust emission. Because the soil PRGs are smaller than the corresponding RBCs, it is not expected that any of the PRGs would pose an acute toxicity hazard by ingestion (see above). The ingestion pathway is a significant driver in the resulting HBESL, though the inhalation pathway is also critical.

The largest PRG for GB is 32 mg/kg soil for a commercial/industrial scenario. At this HBESL and assuming a soil adherence of 0.08 mg per cm<sup>2</sup> of skin and a total exposed skin area of 5700 cm<sup>2</sup>, the total amount of soil on the skin would amount to 456 mg and would contain 0.015 mg of GB. In comparison, experimental studies on humans have shown that 20 mg GB applied to the skin can result in a decrease in blood ChE activity, with no signs or symptoms of toxicity (see Section 1.3.8). A soil PRG of 32 mg/kg soil could theoretically result in a GB air concentration of 0.0002 mg/m<sup>3</sup>, assuming that the air concentration can be estimated from the soil concentration (32 mg/kg) divided by the VF ( $1.7 \times 10^5$  m<sup>3</sup>/kg). In comparison, the estimated no-effect concentration for a 60-min exposure to GB is 0.02 mg/m<sup>3</sup> (see Section 1.3.8).

## 6.3 SOIL SCREENING LEVELS (SSLs)

The equations for calculating USEPA OSWER SSLs (USEPA, 1996a) are given in Section 3.3. The residential soil SSL is identical to the residential soil RBC. For deriving an SSL for inhalation of fugitive dusts in a residential soil, the USEPA default PEF of  $1.32 \times 10^9$  m<sup>3</sup>/kg was applied and the resulting SSL is 4100 mg/kg. This HBESL is presented here only to show the results of the calculation following USEPA's guidelines, and it is not intended as a recommendation for use in remediation. Other SSLs are more protective and must, therefore, take precedence. An SSL was also calculated for inhalation of GB vapors released from soil, in this case using a calculated VF. This SSL is 0.53 mg/kg which is even lower than the PRG value. This is because the SSL model assumes volatility and therefore addresses inhalation of vapors, where the PRG does not (and instead uses a PEF for inhalation of particulate).

An SSL for migration to ground water was not calculated for agent GB. The methodology for this SSL assumes an infinite source and no degradation of agent, conditions which are not likely to apply to GB. The actual potential for agent GB migration to ground water is considered to be quite low (see Appendix E). For this reason, it is recommended that a site-specific analysis be conducted for those situations where ground-water contamination is a concern.



## 6.4 SUMMARY

In this case the SSL methodology yields the most conservative HBESL, primarily due to the assumption regarding volatility. The SSL does not provide a commercial/industrial value; for this scenario the PRG provides a slightly more conservative value than the RBC because of the additive pathways. Still, differences amongst the HBESLs derived from different models are rather small. Though all methods appear to yield appropriate, valid screening values which represent concentrations that do not present acute or chronic health risks for the given scenarios, the PRG method may be used to address the concern of additive toxicity across exposure pathways, and because the differences between approaches are somewhat minimal. The SSL, though more conservative, may overestimate the impact of the inhalation pathway.

## 7. AGENT GA

The HBESLs for agent GA, as derived from the algorithms presented in Section 3, are summarized in Table 7-1. The toxicity values and the environmental parameter values used to calculate the HBESLs are listed in Table 7-2. The exposure parameters used to calculate the RBCs, PRGs and SSLs are described in detail in Sections 2 and 3. The oral RfD for GA is 0.00004 mg/kg/day. The estimated inhalation RfD for GA of  $9 \times 10^{-7}$  mg/kg/day was derived from the DHHS/Army control limit of 0.000003 mg/m<sup>3</sup> by assuming an inhalation rate of 20 m<sup>3</sup>/day and a default body weight of 70 kg. Because there is no evidence that GA is carcinogenic, HBESLs were calculated only for noncarcinogenic effects.

Table 7-1. Summary of calculated HBESLs for agent GA			
Method (units)	Media, Scenario (pathways)	Derived Value	HBESL
			Noncancer only
Region III			
RBC (mg/kg)	Soil, residential (ingestion)		3.1
RBC (mg/kg)	Soil, commercial/industrial (ingestion)		82
Region IX			
PRG (mg/kg)	Soil, residential (ingestion, inhalation, and dermal)		2.8
PRG (mg/kg)	Soil, commercial/industrial (ingestion, inhalation, and dermal)		68
OSWER			
SSL (mg/kg)	Soil, residential (ingestion)	3.1	
SSL (mg/kg)	Soil, residential (inhalation of dusts)	4100	
SSL (mg/kg)	Soil, residential (inhalation of vapors)	0.8	0.8
SSL (mg/kg)	Soil, residential (migration to ground water)	site-specific <sup>a</sup>	

<sup>a</sup> Because the potential for migration to ground water is quite low, it is recommended that a site-specific analysis of this SSL be conducted only for those situations where ground-water contamination is a concern.

Table 7-2. Toxicity values and chemical parameters for agent GA		
Parameter	Value	Units
Oral Reference Dose	0.00004	mg/kg/day
Inhalation Exposure Limit	0.000003	mg/m <sup>3</sup>
Inhalation Reference Dose	0.0000009	mg/kg/day
Dermal absorption factor	0.26 <sup>e</sup>	percent per hr from soil
Vapor pressure <sup>f</sup>	0.07	mm Hg at 25 °C
Water solubility <sup>f</sup>	50-100	g/L
Henry's Law Constant (H) <sup>b</sup>	$1.52 \times 10^{-7}$ g	atm·m <sup>3</sup> /mol
Volatilization factor (VF) <sup>c</sup>	$2.6 \times 10^5$	m <sup>3</sup> /kg
Soil-water partition coefficient (K <sub>d</sub> ) <sup>d</sup>	0.231	
Hydrolysis half-life <sup>a</sup>	8.5	hr, at pH 7, 20 °C
Persistence in soil <sup>a</sup>	1-1.5	days

<sup>a</sup> Value from DA, 1974

<sup>b</sup> Estimated from the ratio of the volatility and the solubility (see Appendix A)

<sup>c</sup> See Appendix A for derivation

<sup>d</sup>  $K_d = K_{oc} \times f_{oc}$ ;  $f_{oc} = 0.006$  g organic carbon/g soil (USEPA default);  $K_{oc}$  = soil organic carbon-water partition coefficient ( $\log K_{oc} = 1.377 + 0.544 \log K_{ow}$ ; where  $K_{ow}$  = octanol-water partition coefficient)

<sup>e</sup> See section 2.3.2.2 and Appendix H

<sup>f</sup> Value from MacNaughton and Brewer, 1994

<sup>g</sup> See Section 2.3.2.4

## 7.1 RISK-BASED CONCENTRATIONS (RBCs)

The equations for calculating USEPA Region III RBCs (USEPA, 1996a) are given in Section 3.1. The soil RBC is based solely on ingestion of contaminated soil. The maximum RBC is 82 mg/kg for the commercial/industrial scenario. At this HBESL, the dose resulting from ingestion of 50 mg of soil is 0.004 mg GA. In comparison, a minimum effect level in humans is estimated to be 0.37 mg (see Section 1.3.8).

## 7.2 PRELIMINARY REMEDIATION GOALS (PRGs).

The equations for calculating USEPA Region IX PRGs (USEPA, 1996b) are given in Section 3.2. Because of its low Henry's Law Constant, agent GA is not expected to volatilize from soil. For the residential and industrial soil PRGs, the  $VF_s$  in the PRG equation is replaced with the particulate emission factor (PEF =  $1.32 \times 10^9 \text{ m}^3/\text{kg}$ ) to account for exposure through fugitive dust emission. Because the soil PRGs are equal to or smaller than the corresponding RBCs, it is not expected that any of the PRGs would pose an acute toxicity hazard by ingestion (see above).

The largest PRG for GA is 68 mg/kg soil for a commercial/industrial scenario. At this HBESL and assuming a soil adherence of 0.08 mg per  $\text{cm}^2$  of skin and a total exposed skin area of  $5700 \text{ cm}^2$ , the total amount of soil on the skin would amount to 456 mg and would contain 0.03 mg of GA. In comparison, it was estimated that the minimum effect level for a percutaneous exposure would be 32-48 mg, and in one experimental human study, a percutaneous dose as high as 400 mg caused no toxic effects but did reduce blood cholinesterase (ChE) activity (see Section 1.3.8). Therefore, the PRG is expected to be protective of any acutely toxic effects under the stated conditions of exposure. A soil PRG of 68 mg/kg soil could theoretically result in a GA air concentration of  $0.0003 \text{ mg}/\text{m}^3$ , assuming that the air concentration can be estimated from the soil concentration (68 mg/kg) divided by the VF ( $2.6 \times 10^5 \text{ m}^3/\text{kg}$ ). In comparison, a no-effect level of  $0.05 \text{ mg}/\text{m}^3$  has been estimated by extrapolation from toxicity data for GB (see Section 1.3.8).

## 7.3 SOIL SCREENING LEVELS (SSLs)

The equations for calculating SSLs (USEPA, 1996c) for GA are given in Section 3.3. The residential soil SSL is identical to the residential soil RBC and is also slightly larger than the residential soil PRG. An SSL for inhalation of fugitive dusts was derived using the USEPA default PEF of  $1.32 \times 10^9 \text{ m}^3/\text{kg}$ , and the DHHS/Army air control limit of  $0.3 \times 10^{-6} \text{ mg GA}/\text{m}^3$  as an RfC. The resulting SSL is 4100 mg/kg. This HBESL is presented here only to show the results of the calculation following USEPA's guidelines, and it is not intended as a recommendation for use in remediation. Other HBESLs are more protective and must, therefore, take precedence. An SSL was also calculated for inhalation of GA vapors released from soil. This SSL is  $0.8 \text{ mg}/\text{kg}$  which is even lower than the PRG value. This is because the SSL model assumes volatility, and therefore addresses inhalation of vapors, where the PRG does not (and instead uses a PEF for inhalation of particulate).

An SSL for migration to ground water was not calculated for agent GA. The methodology for this SSL assumes an infinite source and no degradation of agent, conditions which are not likely to apply to GA. The actual potential for agent GA migration to ground water is considered to be quite low (see Appendices E and H). For this reason, it is recommended that a site-specific analysis be conducted for those situations where ground-water contamination is a concern.

## 7.4 SUMMARY

In this case, the SSL methodology yields the most conservative HBESL, primarily due to assumption regarding volatility. The SSL does not provide a commercial/industrial value. For this scenario the PRG provides a slightly more conservative value than the RBC because of the additive pathways. Still, differences amongst the HBESLs derived from different models are rather small. Though all methods appear to yield appropriate, valid screening values which represent concentrations that do not present acute or chronic health risks for the given scenarios, the PRG method may be used to address the concern of additive toxicity across exposure pathways, and because the differences between approaches are somewhat minimal. The SSL, though more conservative, may overestimate the impact of the inhalation pathway.

## 8. AGENT GD

The HBESLs for agent GD, as derived from the algorithms given in Section 3, are summarized in Table 8-1. The toxicity values and the environmental parameter values that were used to calculate the HBESLs are listed in Table 8-2. The exposure parameters used to calculate the RBCs, PRGs and SSLs are described in detail in Sections 2 and 3. The oral RfD for agent GD is 0.000004 mg/kg/day. The estimated inhalation RfD for GD of  $3 \times 10^{-7}$  mg/kg/day was derived from the DHHS/Army control limit of 0.000001 mg/m<sup>3</sup> by assuming an inhalation rate of 20 m<sup>3</sup>/day and a default body weight of 70 kg. Because there is no evidence that agent GD is carcinogenic, HBESLs were calculated only for noncarcinogenic effects.

Table 8-1. Summary of calculated HBESLs for agent GD			
Method (units)	Media, Scenario (pathways)	Derived Value	HBESL
			Noncancer Only
Region III			
RBC (mg/kg)	Soil, residential (ingestion)		0.31
RBC (mg/kg)	Soil, commercial/industrial (ingestion)		8.2
Region IX			
PRG (mg/kg)	Soil, residential (ingestion, dust inhalation, and dermal)		0.22
PRG (mg/kg)	Soil, commercial/industrial (ingestion, dust inhalation, and dermal)		5.2
OSWER			
SSL (mg/kg)	Soil, residential (ingestion)	0.31	
SSL (mg/kg)	Soil, residential (inhalation of dusts)	4100	
SSL (mg/kg)	Soil, residential (inhalation of vapors)	0.18	0.18
SSL (mg/kg)	Soil, residential (migration to ground water)	site-specific <sup>a</sup>	

<sup>a</sup> Because the potential for migration to ground water is quite low, it is recommended that a site-specific analysis of this SSL be conducted only for those situations where ground-water contamination is a concern.

<b>Table 8-2. Toxicity values and environmental parameters for agent GD</b>		
<b>Parameter</b>	<b>Value</b>	<b>Units</b>
Oral Reference Dose	0.000004	mg/kg/day
Inhalation Exposure Limit	0.000003	mg/m <sup>3</sup>
Inhalation Reference Dose	0.0000003	mg/kg/day
Dermal absorption factor	0.78 <sup>d</sup>	percent per hr from soil
Vapor pressure <sup>a</sup>	0.40	mm Hg
Water solubility <sup>a</sup>	20-30	g/L
Henry's Law Constant (H) <sup>b</sup>	4.56 x 10 <sup>-6</sup>	atm·m <sup>3</sup> /mol
Volatilization factor (VF <sub>s</sub> ) <sup>b</sup>	1.7 x 10 <sup>5</sup>	m <sup>3</sup> /kg
Soil-water partition coefficient (K <sub>d</sub> ) <sup>c</sup>	1.404	NA
Hydrolysis half-life <sup>e</sup>	45	hr at pH 6.65, 25 °C
Persistence in soil	ND	

<sup>a</sup> Value from MacNaughton and Brewer, 1994

<sup>b</sup> See Appendix A

<sup>c</sup>  $K_d = K_{oc} \times f_{oc}$ ;  $f_{oc} = 0.006$  g organic carbon/g soil (USEPA default);  $K_{oc}$  = soil organic carbon-water partition coefficient ( $\log K_{oc} = 1.377 + 0.544 \log K_{ow}$ ; where  $K_{ow}$  = octanol-water partition coefficient)

<sup>d</sup> See section 2.3.2.2 and Appendix H

<sup>e</sup> Value from DA, 1974

## 8.1 RISK-BASED CONCENTRATIONS (RBCs)

The equations for calculating USEPA Region III RBCs (USEPA, 1996a) are given in Section 3.1. The soil RBC is based solely on ingestion of contaminated soil. The maximum RBC is 8.2 mg/kg for a commercial/industrial scenario. At this HBESL, the dose resulting from ingestion of 50 mg of soil is 0.0004 mg GD. In comparison, a minimum effect level in humans is estimated to be 0.09 mg for oral exposures (see Section 1.3.8).

## 8.2 PRELIMINARY REMEDIATION GOALS (PRGs)

The equations for calculating USEPA Region IX PRGs (USEPA, 1996b) are given in Section 3.2. Because of its low Henry's Law Constant, agent GD is not expected to volatilize from soil. Therefore, the  $VF_s$  in the PRG equation is replaced with the particulate emission factor ( $PEF = 1.32 \times 10^9 \text{ m}^3/\text{kg}$ ) to account for exposure through fugitive dust emission. Because the soil PRGs are equal to or smaller than the corresponding RBCs, it is not expected that any of the PRGs would pose an acute toxicity hazard by ingestion (see above).

The largest PRG for GD is 5.2 mg/kg soil for a commercial/industrial scenario. At this HBESL and assuming a soil adherence of 0.08 mg per  $\text{cm}^2$  of skin and a total exposed skin area of  $5700 \text{ cm}^2$ , the total amount of soil on the skin would be 456 mg and would contain 0.002 mg of GD. In comparison, it has been estimated that the minimum effect levels for percutaneous exposures is 11 mg (see Section 1.3.8).

A soil PRG of 5.2 mg/kg soil could theoretically result in a GD air concentration of  $0.00005 \text{ mg/m}^3$ , assuming that the air concentration can be estimated from the soil concentration (5.2 mg/kg) divided by the VF ( $1.7 \times 10^5 \text{ m}^3/\text{kg}$ ). In comparison, a no-effect level of  $0.013 \text{ mg/m}^3$  has been estimated by extrapolation from toxicity data for GB (see Section 1.3.8).

## 8.3 SOIL SCREENING LEVELS (SSLs)

The equations for calculating SSLs (USEPA, 1996c) for GD are given in Section 3.3. An SSL for inhalation of fugitive dusts was derived using the USEPA default PEF of  $1.32 \times 10^9 \text{ m}^3/\text{kg}$ , and the DHHS/Army air control limit of  $0.3 \times 10^{-6} \text{ mg/m}^3$  as an RfC. The SSL for inhalation of GD vapors, as derived using the VF of  $1.7 \times 10^5 \text{ m}^3/\text{kg}$ , is 0.18 mg/kg. This SSL value is even lower than the PRG value. This is because the SSL model assumes volatility, and therefore addresses inhalation of vapors, where the PRG does not (and instead uses a PEF for inhalation of particulates).

An SSL for migration to ground water was not calculated for agent GD. The methodology for this SSL assumes an infinite source and no degradation of agent, conditions which are not likely to apply to GD. The actual potential for agent GD migration to ground water is considered to be quite low (see Appendix E). For this reason, it is recommended that a site-specific analysis be conducted for those situations where ground-water contamination is a concern.



## 8.4 SUMMARY

In this case the SSL methodology yields the most conservative HBESL, primarily due to assumption regarding the volatility. The SSL does not provide a commercial/industrial value; for this scenario the PRG provides a slightly more conservative value than the RBC because of the additive pathways. Still, differences among the HBESLs derived from different models are rather small. Though all methods appear to yield appropriate, valid screening values which represent concentrations that do not present acute or chronic health risks for the given scenarios, the PRG method may be used to address the concern of additive toxicity across exposure pathways, and because the differences between approaches are somewhat minimal. The SSL, though more conservative, may overestimate the impact of the inhalation pathway.

## 9. Lewisite

The HBESLs for Lewisite, as derived from the algorithms given in Section 3, are summarized in Table 9-1. The toxicity values and the environmental parameter values that were used in their derivation are listed in Table 9-2. The exposure parameters used to calculate the RBCs, PRGs and SSLs are described in detail in Sections 2 and 3. The oral RfD for Lewisite is  $0.1 \mu\text{g/kg/day}$ . The estimated inhalation RfD of  $0.00086 \text{ mg/kg/day}$  was derived from the DHHS/Army control limit of  $0.003 \text{ mg/m}^3$  by assuming an inhalation rate of  $20 \text{ m}^3/\text{day}$  and a default body weight of  $70 \text{ kg}$ .

Table 9-1. Summary of calculated HBESLs for Lewisite <sup>a</sup>			
Method (units)	Media/Scenario (pathways)	Derived Value	HBESL
			Noncancer Only
Region III			
RBC (mg/kg)	Soil, residential (ingestion)	7.8	7.8
RBC (mg/kg)	Soil, commercial/industrial (ingestion)	200	(7.8) <sup>b</sup>
Region IX			
PRG (mg/kg)	Soil, residential (ingestion, inhalation, and dermal)	0.3	0.3
PRG (mg/kg)	Soil, commercial/industrial (ingestion, inhalation, and dermal)	3.7	3.7
OSWER			
SSL (mg/kg)	Soil, residential (ingestion)	7.8	7.8
SSL (mg/kg)	Soil, residential (inhalation of dusts)	4.1 x 10 <sup>6</sup>	
SSL (mg/kg)	Soil, residential (inhalation of vapors)	NA <sup>c</sup>	
SSL (mg/kg)	Soil, residential (migration to ground water)	NA <sup>d</sup>	

<sup>a</sup> Because of rapid hydrolysis, these HBESLs also apply to the degradation product, 2-chlorovinylarsonous acid.

<sup>b</sup> RBC value derived for the commercial/industrial scenario was potentially above acute toxicity levels, therefore the upper bound value of the residential scenario is suggested as a substitute.

<sup>c</sup> SSL cannot be calculated because a Volatilization Factor is not available

<sup>d</sup> SSL cannot be calculated because a  $K_{ow}$  is not available

Although Lewisite is a suspect carcinogen because it is an arsenic-based compound (inorganic arsenic has been classified as a known human carcinogen), there are no epidemiological or experimental data verifying its carcinogenicity or quantifying its carcinogenic potency (there are no oral or inhalation slope factors). Therefore, HBESLs for Lewisite are derived here only for noncarcinogenic endpoints. It is

recommended, however, that existing EPA screening levels for inorganic arsenic be used for carcinogenic endpoints.

An experimentally derived skin absorption factor (ABS) is not available for Lewisite; therefore, a default value of 0.1 is used in accordance with USEPA Region IX guidelines for organic compounds (USEPA 1996b). Also, the oral RfD for Lewisite was not applied directly as a dermal RfD, though this procedure is often used by EPA Region IX in absence of a dermal RfD. As described previously, the median threshold dose for blistering has been reported to be 14 µg and a dose as low as 3.5 µg reportedly caused erythema in 27 out of 93 individuals and blisters in 8 of the 93 (see Section 1.3.8). Because the standard methodology (using the oral RfD applied as a dermal RfD) results in a dermal RfD (of 4 µg) which is above a potential dermal effect level, the Lewisite HBESLs were calculated using a dermal RfD based on the existing acute dermal toxicity data which results in an more conservative estimate. Calculations are described in section 9.2 below.

<b>Table 9-2. Toxicity values and environmental parameters for Lewisite</b>		
<b>Parameter</b>	<b>Value</b>	<b>Units</b>
Oral Reference Dose	0.0001	mg/kg/day
Inhalation Exposure Limit	0.003	mg/m <sup>3</sup>
Inhalation Reference Dose	0.0009	mg/kg/day
Dermal Reference Dose <sup>d</sup>	0.0000017	mg/kg/day
Dermal absorption factor	10	percent
Vapor pressure <sup>a</sup>	0.58	mm Hg
Water Solubility (WS)	0.5 <sup>b</sup>	g/L
Henry's Law Constant (H)	NA <sup>b</sup>	atm m <sup>3</sup> /mol
Volatilization factor (VF <sub>s</sub> )	NA <sup>b</sup>	m <sup>3</sup> /kg
Soil-water partition coefficient (K <sub>d</sub> )	NA <sup>b</sup>	NA
Hydrolysis half-life	Rapid <sup>c</sup>	
Persistence in soil	"Intermediate" <sup>c</sup>	days

<sup>a</sup> Value from MacNaughton and Brewer, 1994

<sup>b</sup> Because of rapid hydrolysis, estimates of water solubility are not meaningful (Rosenblatt et al., 1975); H, VF and K<sub>d</sub> cannot be derived

<sup>c</sup> DA, 1974

<sup>d</sup> Derived from acute toxicity data (see Section 9.2)

## 9.1 RISK-BASED CONCENTRATIONS (RBCs)

The equations for calculating USEPA Region III RBCs (USEPA, 1996a) are given in Section 3.1. The soil RBC is based solely on ingestion of contaminated soil. The maximum RBC is 200 mg/kg for a commercial/industrial scenario. At this HBESL, the dose resulting from ingestion of 50 mg of soil is 0.01 mg. Experimentally derived minimum effect levels (MELs) in animals range from 0.07 to 2 mg/kg (see Section 1.3.8), equivalent to 0.02 - 0.6 mg per animal. Other data (described below) suggest acute dermal effects at lower dose levels. In all, the HBESL derived for the commercial/industrial scenario appears to be at a level where acute effects could potentially be exhibited under the assumed exposure conditions. Though the limited data do not permit a clear demarcation of what level acute effects would occur, the concern should not be overlooked. For purposes of this document, the HBESL resulting from the RBC *residential* calculation (7.8 mg/kg) is also recommended for application in a commercial/industrial scenario.

At a concentration of 7.8 mg of Lewisite/kg of soil, ingestion of 50 mg of soil yields 0.004 mg Lewisite; a dose which is lower than the estimated MELs.

## 9.2 PRELIMINARY REMEDIATION GOALS (PRGs)

Because the standard EPA Region methodology in which the oral RfD is applied as a dermal RfD results in a dermal Lewisite RfD of 7  $\mu\text{g}$ , which is above a potential dermal effect level, the Lewisite HBESLs were calculated using a dermal RfD based on the existing acute dermal toxicity data which results in a more conservative estimate. This was accomplished by adjusting the reported effect level of 3.5  $\mu\text{g}$  (see Section 1.2) by a standard factor of 10 to arrive at an estimated no-effect level of 0.35  $\mu\text{g}$ . Because dose-response data are not available to be certain that 0.35  $\mu\text{g}$  is a no-effect level, an additional Modifying Factor of 3 was applied, resulting in a value of 0.12  $\mu\text{g}$ . For a 70 kg person this is equivalent to a dose of 0.0017  $\mu\text{g}/\text{kg}$  body weight (0.0000017 mg/kg). This value was then used as the dermal RfD in the PRG equation. The resulting commercial/industrial HBESL calculated for Lewisite is therefore 3.7 mg/kg. Assuming a soil adherence of 0.08 mg per  $\text{cm}^2$  of skin (USEPA default) and a total exposed skin area of 5700  $\text{cm}^2$ , the total amount of soil on the skin at the HBESL would be 456 mg and would contain 1.7  $\mu\text{g}$  of Lewisite ( $0.08 \text{ mg}/\text{cm}^2 \times 5700 \text{ cm}^2 = 456 \text{ mg} \times (3.7 \text{ mg}/\text{kg}/1000000) = 0.0017 \text{ mg} = 1.7 \mu\text{g}$  Lewisite). Under the exposure assumptions used to derive the HBESL of 3.7, the total dose of 1.7  $\mu\text{g}$  would be dispersed over a surface area of 5700  $\text{cm}^2$ , resulting in an average exposure per unit of exposed surface area of 0.0003  $\mu\text{g}/\text{cm}^2$  (i.e., 1.7  $\mu\text{g}$  Lewisite / 5700  $\text{cm}^2$ ). It is assumed that this exposure does not occur at a single point in time but rather over a period of time during the day. Therefore, it is unlikely that acutely toxic effects would occur at this HBESL level of 3.7 mg/kg. *It must be kept in mind that the effect level (3.5  $\mu\text{g}$ ) is for pure agent concentrated in a single small area of the skin; whereas, the PRG methodology assumes an even dispersion of the agent throughout the soil. Obviously, the soil PRGs for vesicants such as Lewisite would not apply if the agent is clumped into discrete masses.*

### 9.3 SOIL SCREENING LEVELS (SSLs)

The equations for calculating USEPA OSWER SSLs (USEPA, 1996a) are given in Section 3.3. An SSL for inhalation of fugitive dusts was derived using the USEPA default PEF of  $1.32 \times 10^9 \text{ m}^3/\text{kg}$ , and the DHHS/Army air control limit of  $0.003 \text{ m}^3/\text{m}^3$  as an RfC. The resulting SSL is  $4.1 \times 10^6 \text{ mg/kg}$ . This HBESL is presented here only to show the results of the calculation following USEPA's guidelines, and it is not intended as a recommendation for use in remediation. Other HBESLs are more protective and must, therefore, take precedence. A SSL for inhalation of vapors could not be calculated due to data limitation. An SSL for migration to ground water cannot be calculated for Lewisite because of its instability in water. The SSL for the ingestion pathway,  $7.8 \text{ mg/kg}$ , as always is identical to the residential RBC value. As stated above, this level should be protective against both chronic and acute effects; however, there is uncertainty due to data limitations. Finally, as in the case of the RBCs and PRGs, one should consider CVA (see Appendix F) for screening purposes where Lewisite is a concern.

### 9.4 SUMMARY

PRGs are the most protective HBESLs for Lewisite, because they incorporate multipathway exposures and specifically allow one to address the dermal pathway and acute toxicity concerns. As noted in Section 1.3.7, PRGs may be overly conservative where toxic effects of a chemical are not expected to be additive across pathways, as is the case of vesicants such as Lewisite, where the primary toxic effect is at the point of contact. However, if acute toxicity is a concern this is irrelevant. In addition, there is evidence that Lewisite may be absorbed systemically even at low doses; therefore, that PRGs may be the most appropriate model to use for this agent. It is also recommended that if rapid degradation of Lewisite is expected, screening levels for the primary degradation product of Lewisite, CVA/Lewisite oxide, be included in the screening process.

## 10. COMPARISON OF SCREENING METHODS

The screening approaches for soil contamination used by OSWER and USEPA's Regional Offices differ in varying degrees. In all, these approaches encompass single and multiple exposure pathways including ingestion, dermal contact, inhalation of dusts, inhalation of volatiles, and migration to ground water. This section identifies the similarities and differences in these methods by discussing the individual exposure routes, and summarizes their appropriateness for conducting risk assessments for chemical warfare agents.

### 10.1 Ingestion

USEPA Region III residential soil RBC is identical to the OSWER surface soil screening level in that both are limited to one exposure pathway, that of soil ingestion by children. Either of these HBESLs are appropriate for environmental contaminants that are nonvolatile and have a low potential for dermal absorption. If a contaminant is volatile, it is less likely to pose a significant risk through dermal contact unless its adsorption to soil particles limits volatilization. However, all the agents discussed in this report have relatively low soil adsorption coefficients (see Table 2-3); therefore, binding to soil is not expected to be significant. For the vesicants which have dermal effects, and for agent VX which is considered nonvolatile and is readily absorbed through the skin, any screening levels based on soil ingestion alone should be compared to screening levels based on potential dermal contact with the contaminants.

### 10.2 Dermal

While USEPA Region III RBCs do not directly address the dermal exposure route, it does (USEPA, 1995a) support the use of the method given in the Superfund Risk Assessment Guidance Document (USEPA, 1989) for estimating dermal exposures. This method can be used to derive a soil screening level specifically for dermal exposures to contaminated soil. Dermal exposures can be estimated from information on the amount of skin surface area exposed, the soil-to-skin adherence factor, and the dermal absorption factor. The estimated absorbed dose is then compared to a dermal RfD to derive the screening level. This approach is equivalent to the dermal exposure *component* of Region IX's soil PRGs for residential and industrial/commercial scenarios. By direct implementation, only the Region IX screening levels directly incorporate this pathway.

Two key factors are used to derive a dermal screening level; the dermal absorption factor and the dermal RfD. The dermal absorption factor is a chemical-specific value which allows for the estimation of the absorbed dose. USEPA Region III has summarized the available pertinent information on dermal absorption values for a range of volatile and semivolatile organic compounds and has recommended a conservative default value of 10% for semivolatile organic compounds and pesticides (USEPA, 1995a). Similar defaults

are used by USEPA Region IX. However, USEPA Region IV recommends 1% as the default for organic compounds (and 0.1% for inorganics) on the basis that skin absorption will be reduced due to binding of the chemicals to the soil. Volatile chemical agents such as the G agents are unlikely to pose a dermal hazard; however, the risks from dermal exposure to VX and HD may be significant. Theoretical estimates of skin absorption of chemical warfare agents in a soil matrix range from 0.27%/hr for VX to 0.70%/hr for HD (Majors, 1997). Based on these estimates, chemical-specific 8-hour cumulative dermal absorption factors were used to calculate industrial soil PRGs and 12-hour cumulative dermal absorption factors were used to calculate soil PRGs for residential and trespasser exposures. These values (see Table 2-4) fall between the 1% default recommended by Region IV and the 10% default recommended by Region IX.

The second key component for deriving a soil screening level for dermal exposures is the dermal RfD. Dermal RfDs for chronic or subchronic exposures are not available for any of the chemical warfare agents. For systemic toxins, a dermal RfD is the equivalent of an absorbed dose RfD and can be estimated from the oral RfD by the use of a chemical-specific gastrointestinal absorption factor. This approach is applicable to the nerve agents which are systemic toxins; however, insufficient data were available to estimate gastrointestinal absorption factors. USEPA Region IX states that, in the absence of chemical-specific gastrointestinal absorption data, the oral RfD can be used in place of the estimated dermal RfD (i.e., a gastrointestinal absorption rate of 100% is assumed). This is the general approach used in this report.

If the effects are localized, and not the result of systemic uptake, as in the case of vesicants, a dermal RfD is more likely to be a function of applied dose rather than the absorbed dose. Thus, for vesicants HD and Lewisite, a dose per unit area of skin may be a more appropriate dermal RfD to compare with the potential skin exposures. Such dermal RfDs are not available for these agents. It should be noted, however, that the critical effect seen in animal toxicity studies on which the oral RfDs for both HD and Lewisite were based, involved pathological changes in the epithelial surface of the gastrointestinal tract, consistent with the vesicant properties of these compounds. For HD, the oral RfD was used instead of a dermal RfD - and the resulting screening levels compared with available data. For Lewisite, comparisons of available acute dermal data suggested that use of the oral RfD was inadequate; therefore a dermal RfD was calculated.

### 10.3 Migration to Ground Water

The OSWER soil screening level for potential migration of a contaminant to ground water is dependent on a set of simplifying conditions (see Section 3.3.7) including the assumption of an infinite source, uniform distribution in soil, and no attenuation in soil or ground water. It is unlikely that these conditions will be maintained for any of the chemical warfare agents discussed in this report. The agents are likely to occur only in very limited areas and most are very susceptible to hydrolysis and degradation to less toxic forms. This is particularly true for the nerve agents GA, GB, and GD, whose persistence in soil is usually measured in days (see Section 1.2.3). Agent VX is expected to be more persistent in soils than the G agents because it is relatively nonvolatile and less susceptible to hydrolysis. VX is water soluble (10-50 g/L), and has a relatively low potential for soil adsorption ( $K_d = 1.962$  for soils with organic carbon level of 0.006

g/g: see Table 2-3). Therefore, VX would also be expected to have a greater potential for migration to ground water than the G agents. However, it should be noted that laboratory studies indicate that 90% of VX was degraded after only 2 days when tested in three types of soil [(humic sand, humic loam, and clayey peat (Verweij and Boter, 1976)]. These data indicate that there is little potential for migration to ground water for any of the nerve agents (GA, GB, GD or VX). USEPA notes that for contaminants at sites with shallow sources, thick unsaturated zones, degradable contaminants, or unsaturated zone characteristics (e.g., clay layers), the concentrations of the contaminants may be reduced substantially before they reach the ground water (USEPA, 1996d). In such cases, USEPA recommends the use of unsaturated zone models for soil screening. These models, which are described in more detail in the Technical Background Document (USEPA, 1996d) of the Soil Screening Guidance, may be relevant for environmental screening of the chemical warfare agents. Furthermore, USEPA recommends that mass-limit SSLs be calculated when the area and depth of a contaminated soil source is known, or can be estimated with confidence. The equation for deriving mass-limit SSLs is given in Section 3.3.7.3. Mass-limit SSLs may be more appropriate for the chemical warfare agents than generic ground-water SSLs based on the assumptions mentioned above.

The low potential for the nerve agents to migrate to ground water is supported by the results of the ground-water modeling exercises described in Appendix E. Unlike the SSL approach, these models used information on the rates of agent degradation through hydrolysis.

Agent HD may remain in subsurface soils for years when undisturbed: individual droplets (micelles) of this agent are likely to be encased with a polymeric coating (formed from unhydrolyzed agent and its primary degradation product, thiodiglycol), which prevents further dissolution of the agent into the surrounding soil. In this form, migration of HD to ground water would be unlikely. In addition, any mustard dissolving from such micelles would be subject to rapid hydrolysis since the hydrolysis half-life of dissolved HD agent is less than 10 minutes at environmental temperatures (see Table 1-1). Results of the ground-water modeling exercises described in Appendix E also indicate a very low potential for ground-water contamination by HD.

In the case of Lewisite, this agent is subject to rapid hydrolysis to CVA. Therefore, SSLs for migration to ground water for Lewisite should be based on CVA (see Appendix F).



## 10.4 Airborne Dust

The OSWER has developed a separate soil screening level for inhalation of contaminated soil particles resuspended in air. This SSL incorporates a default particulate emission factor (PEF, see Section 2.3.3.2) that is dependent on wind speed and vegetative cover. This HBESL results in very high soil values because it assumes that only a small fraction of the contaminated soil will be suspended as dust and inhaled. USEPA states that SSL for inhalation of fugitive dust does not need to be routinely calculated for organic compounds because of the strong likelihood that the ingestion SSL would be more protective. For acutely toxic chemicals such as the warfare agents, the high dust SSL may exceed acutely toxic levels. Therefore, it is unlikely that the SSL for inhalation of dusts will ever be used as an HBESL. Other HBESLs (or PRGs or RBCs) are more conservative and would be used instead. Furthermore, in the case of vesicants, contact of the contaminated dusts with the eyes or skin may pose as great a potential hazard as inhalation of the dusts; therefore, this SSL may greatly underestimate potential risks associated with exposure to nonvolatile vesicant agents.

## 10.5 Volatiles

The SSL for inhalation of volatile contaminants released from subsurface soils incorporates a chemical-specific VF (see Section 2.3.2.4) that is dependent on the chemical's diffusivity in air and water, its Henry's Law Constant, and its soil adsorption coefficient, as well as several soil characteristics. The VF is derived from a model that calculates the maximum flux of the contaminant from a soil based on soil moisture conditions and on the air-filled soil porosity. It assumes an infinite contaminant source and vapor phase diffusion as the only transport mechanism. Because contaminant sources for chemical warfare agents are likely to be very limited, this SSL may not be applicable to the agents, and the values presented in this report may *overestimate* the potential risks. The OSWER recommends the mass-limit approach when information about the size of the source is known (see Section 3.3.5.1), and it is recommended that this approach be used for chemical warfare agents on a site-specific basis whenever possible.

## 10.6 Multipathway

USEPA Region IX residential and industrial soil PRGs incorporate three exposure pathways, ingestion of soil, inhalation of volatiles (or particulates) released from soil, and dermal absorption following skin contact (see Sections 3.2.3-3.2.6). For a noncancer endpoint, the residential soil PRG is calculated for a child only. The soil ingestion component of the PRG is identical to residential soil RBC for Region III and the residential soil SSL derived by OSWER. In the inhalation component of the PRG, the Henry's Law Constant (H) of a contaminant is used to determine whether the inhalation pathway is a significant source of exposure, as in the case of the tapwater RBCs and PRGs. Chemicals with an H of  $10^{-5}$  atm-m<sup>3</sup>/mol or less and a molecular weight of more than 200 are not considered to pose an inhalation risk. Based on this definition, HD is the only chemical warfare agent, of those considered in this report, that is expected to be an

inhalation hazard from contaminated soils. In most soils, however, hydrolysis (half-life 8.5 minutes) is likely to limit the amount of HD released through volatilization.

If volatilization is considered significant for any soil contaminant, a chemical-specific VF is used in the Region IX soil PRG equation. This VF is derived in an identical manner to that used by OSWER to estimate a VF for use in calculating an SSL for inhalation of volatile organics, and it is subject to the same limitations. A major limitation is the assumption that there is an infinite contaminant source and that vapor phase transport is the only transport mechanism. These assumptions are not likely to apply to the chemical warfare agents which are expected to occur in only limited quantities and may be subject to degradation. Furthermore, the VF is derived from a set of chemical-specific parameters (e.g., air and water diffusivity, Henry's Law Constant, and soil adsorption coefficients). In the case of the chemical warfare agents, most of these parameters were not determined experimentally, but were estimated using predictive models (see Appendix A). Therefore, the derived values and the resultant VFs for the agents, as presented in Table 2-3, have a high level of uncertainty associated with them, and this uncertainty can only be reduced by experimental verification.

If volatilization is not considered significant for any specific contaminant, the Region IX PRG method incorporates a default PEF that accounts for exposures through inhalation of fugitive dusts. This default PEF is identical to that used by OSWER for calculating an SSL for fugitive dusts. Because the PEF is quite large ( $1.32 \times 10^9 \text{ m}^3/\text{kg}$ ), it has an insignificant effect on the final values when used in the PRG equation. In such cases, the ingestion and dermal pathways are the determining factors.

The dermal portion of the Region IX PRG for residential or industrial soils is identical to the approach used in the Superfund Risk Assessment Guidance for estimating dermal exposures (USEPA, 1989). USEPA Region IX allows for the use of the oral RfD as a surrogate dermal RfD if chemical-specific information on gastrointestinal absorption rates is not available. This is the approach followed in this report.

The use of soil PRGs for HBESLs may be considered most appropriate in those cases where the target organ is the same for each exposure pathway and the effects are expected to be additive. For systemically absorbed compounds, such as the nerve agents VX, GA, GB, and GD, it is usually assumed that the effects are additive across pathways. Therefore, PRGs would be the most appropriate HBESLs. For vesicant agents, different exposure pathways may affect different epithelial tissues and the effects are not likely to be additive. Therefore, for HD and Lewisite, pathway-specific screening levels (RBCs or SSLs) may be more appropriate than some PRGs.

## 11. SUMMARY AND RECOMMENDATIONS

### 11.1 GENERAL

Environmental screening levels (referred to by different names by the various USEPA Regions) are low-level concentrations of individual chemicals in environmental media, which, if not exceeded, are unlikely to present a human health hazard for specific exposure scenarios. These 'low-level' concentrations are back-calculated from various USEPA risk assessment models using predetermined, conservative "acceptable risk" quantifiers. These screening levels have been calculated for hundreds of commercial chemicals that are presumed to present potential environmental health impacts at sites where soil has been contaminated. Chemical warfare agents, as chemicals that may be identified as environmental contaminants, may be evaluated with the same health risk assessment methodologies.

During the initial evaluation phase of an environmental health risk assessment, these pre-established environmental screening levels for chemical compounds can aid the assessment process by their use as "action or no-action" determinant criteria. For a specified type of scenario, if the actual soil concentrations were to fall below the established screening level, no further "action" would be deemed necessary. If concentrations were above the screening level, additional "action" would be necessary. This "action" requirement may be met by a variety of procedures to include: performing a detailed site-specific health risk assessment; applying management controls to minimize exposure; implementing treatment/remedial operations; or a combination of these options. By focusing assessment efforts in this manner, screening levels can help to optimize resources and minimize unnecessary expenditures of time and money.

Another benefit of pre-established environmental screening levels is that they allow a means to determine whether analytical detection capabilities for chemical contaminants are adequate. This is particularly beneficial if the compounds are very toxic and the resulting screening levels are extremely low.

These benefits have been demonstrated by the generation and use of screening levels for a wide variety of commercial/industrial contaminants by different USEPA and state regulatory agencies and the responsible regulated communities and industries. The screening approach can reasonably provide similar benefits for those parties involved with determining future action requirements at sites contaminated by unique military compounds such as the chemical warfare agents HD, Lewisite, GA, GB, GD, and VX.

In recommending a set of pre-established HBESLs, however, methodology variations, scientific data limitations and inconsistencies, and risk management issues must be carefully evaluated. Most of these same considerations must be evaluated in detail during site-specific or 'baseline' risk assessments. For screening purposes, some additional degree of 'conservatism' (resulting in media concentrations potentially lower than what might actually pose a significant public health hazard) is necessary than when performing a baseline site-specific risk assessment.

## 11.2 REVIEW OF SCREENING METHODS

### 11.2.1 EPA Region III Risk-Based Concentrations (RBCs)

RBCs may be acceptable screening levels in those cases where the effects of a compound are not expected to be additive or cumulative across exposure pathways. This may be particularly true for low-level exposures to vesicants if there is no systemic absorption and the critical effect occurs at the point of contact. However, soil RBCs pertain only to the ingestion pathway, and for vesicants or agents that are readily absorbed through the skin, the soil RBCs may underestimate the potential hazard. Dermal exposures should be evaluated when the chemical characteristics or toxicity of a chemical warrant it.

For systemically absorbed contaminants such as the nerve agents, particularly those that exert their toxic effect on the same physiological system regardless of the exposure pathway, RBCs are likely to underestimate the potential hazard.

### 11.2.2 Region IX Preliminary Remediation Goals (PRGs)

Because soil PRGs incorporate multiple exposure pathways (ingestion, skin contact, and inhalation), they result in lower screening values than the soil RBCs. The appropriateness of the PRGs is contingent on several factors to include: whether all exposure pathways are relevant for a given contaminant, whether the same toxic endpoint occurs regardless of the exposure route, and whether toxicity values (RfDs and/or slope factors) are available for each exposure route or whether they can reasonably be estimated from the ones that are available. In situations where the toxicity endpoints may be different for each exposure pathway, as in the case of the vesicants HD and Lewisite, PRGs may theoretically result in overly conservative HBESLs - however, acute toxicity evaluation should be considered.

The soil PRGs take into account the possibility of inhalation exposures resulting from volatilization of a chemical from subsurface soil (PRGs do not apply to surface spills). According to USEPA Region IX, a chemical's Henry's Law Constant, which is the ratio of its volatility to its water solubility, can be used to determine whether volatilization results in a significant inhalation exposure. As discussed by USEPA (1996d), subsurface volatilization is a function of soil moisture and the partitioning of the chemical between soil pore water and soil pore air (as reflected in a chemical's Henry's Law Constant). Chemicals with a Henry's Law Constant less than  $1 \times 10^{-5}$  atm-m<sup>3</sup>/mol and a molecular weight greater than 200 are not expected to volatilize from subsurface soils (USEPA, 1996b), presumably because the chemical will partition primarily to soil pore water.

If USEPA Region IX's approach is followed, none of the nerve agents would be expected to volatilize from subsurface soils because their Henry's Law Constants are below  $1 \times 10^{-5}$  atm-m<sup>3</sup>/mol. This conclusion is counterintuitive for a chemical such as agent GB which has a relatively high vapor pressure (2.9 mm Hg at 25 °C). Although this may be partially explained by the fact that GB is totally miscible in water, there nevertheless remains some degree of uncertainty surrounding the assumption that GB will not volatilize from

subsurface soil, particularly from relatively dry soil. For arid conditions, a soil PRG can be calculated for GB using its chemical-specific soil VF. Although the Henry's Law Constant for HD is slightly above  $1 \times 10^{-5}$  atm-m<sup>3</sup>/mol, its tendency to encapsulate, and quickly hydrolyze when dissolved, is expected to minimize volatilization from subsurface soils. Similarly, Lewisite hydrolyzes rapidly to a nonvolatile product; therefore, volatilization from subsurface soils is not expected to be environmentally relevant.

Where toxicity data exist for specific agents, the predicted levels of exposure at the PRG-derived HBESLs were compared with minimum effect levels for acute toxicity. These calculations indicated that the potential for acutely toxic exposures was low. These estimates were based on certain assumed and plausible conditions of exposure, and do not include all possible exposure situations.

### 11.2.3 EPA OSWER Soil Screening Levels (SSLs)

The SSL for ingestion of surface soils is derived in a manner identical to that for residential soil RBCs. Both methods are conservatively based on potential exposures to children, considered to be the most susceptible receptor.

The SSLs for inhalation of dusts released from surface soils and for inhalation of volatiles released from subsurface soils, are single pathway screening levels. The SSL for dusts uses a default particulate emission factor that results in extremely high SSL values. As mentioned previously, these SSLs are calculated only to show the results of following USEPA's guidelines; they are not a recommendation for use.

The SSLs for inhalation of volatiles released from subsurface soils is identical to the inhalation component of the soil PRG. It should be noted that this refers to low concentrations of contaminants in subsurface soils, assumes an infinite source of contamination, and requires the calculation of a chemical-specific Volatilization Factor (see Appendix A). When the source is limited, and the size and depth of the contaminated area is known, USEPA recommends deriving a mass-limit SSL with a mass-limit VF (see Section 3.3.5). Mass-limit SSLs are likely to be relevant for chemical agents which are not expected to be widely dispersed and should be calculated whenever site-specific data are available.

The SSLs for migration of contaminants from subsurface soils to ground water requires the use of a set of simplifying assumptions. These assumptions are not likely to apply to the chemical warfare agents because of their expected highly localized distribution in the soil, their relatively rapid degradation, or their expected immobility (HD). Mathematical modeling indicates that the likelihood of any agent migrating to ground water is very low (see Appendix E). For this reason, SSLs for migration to ground water were not calculated for any of the agents. It is recommended that if necessary, ground-water SSLs be evaluated on a site-specific basis.

### 11.3 CONCLUSIONS

**11.3.1** The three EPA methods assessed are very similar; the differences do not generally yield substantially different screening levels. The additive pathway approach incorporated by the PRG Region IX generally results in some of the more conservative (lower) values, primarily due to the additive effects of the inhalation route, and to some degree the dermal route. The SSL inhalation pathway model also produces some of the most conservative values. For the vesicants HD and L, the RBC model must be used cautiously to ensure resulting concentrations do not yield acute effects. In all, the “best” model may be different for different chemicals and situations. The benefits and disadvantages of one method over another are somewhat speculative, but depend on chemical and site/exposure-specific considerations. Ultimately, stakeholders (including site regulators, the public and Army personnel) must evaluate the available information to determine whether the use of a screening approach is warranted and, if so, what models and parameters best suit the situation.

**11.3.2** The HBESL values calculated in this document are intended to represent conservative values for use in *screening* contaminated sites for potential human health risks. The degree of ‘conservatism’ that is truly represented cannot be quantified due to the uncertainties inherent to the risk assessment models. These uncertainties are further compounded by limited data regarding both the chemical warfare agents and the human exposure process. A limitation of the application of the HBESLs for generic scenarios is that, by using a standardized approach and assumptions, unique site-specific variables may be overlooked. Therefore, before application of HBESLs as action/no-action determinants, the user must first evaluate the situation to ensure that certain assumption criteria are met. This includes ensuring that all stakeholders have input to the application of screening levels. However, despite the weaknesses associated with deriving and applying HBESLs, they provide a mechanism to make efficient, consistent, and scientifically based action/no-action decisions when assessing the potential for chronic health effects to exposed populations.

**11.3.3** HBESLs are derived on the assumption that exposure will be of chronic duration, which according to USEPA covers a time span of 7 years to a lifetime. However, empirical data and theoretical estimates indicate that soil persistence of the nerve agents is likely to be no more than several months even under the worst-plausible conditions. Current EPA models do not consider environmental degradation; it is therefore quite possible that actual exposure durations/frequencies are significantly overestimated resulting in conservatively “safe” screening levels. This complex issue of degradation should be considered in chemical and site-specific evaluations when using screening levels and may need to be more critically incorporated in a site-specific risk assessment. Depending on many factors - including (but not limited to) environmental conditions and quantities released - persistence of the agent HD in soils could potentially be measured in years (refer to section 1.2.3), mainly as a result of the agent being encapsulated in an inert polymeric coating formed by its hydrolysis products. As noted previously, HBESLs are not applicable to such situations because acutely toxic exposures are possible if such capsules are broken. Soil persistence data for Lewisite are not available; however, the literature indicate that Lewisite would degrade rapidly to CVAA/ Lewisite oxide, which would eventually degrade to inorganic arsenic. CVAA and Lewisite oxide are presumed to be somewhat persistent, however, and as toxic as their parent compound. Screening levels are available for these degradation products (see Appendix F). Of the other chemical warfare agents evaluated in this report,

only agent VX degrades to a toxic and potentially persistent compound, S-(Diisopropylaminoethyl) methylphosphonothioate (EA-2192). The HBESLs derived for VX can also be used for this compound (see Appendix F). In the cases of Lewisite and VX, assessments for the presence of breakdown compounds Lewisite oxide and inorganic arsenic (for Lewisite) and EA-2192 (for VX) are warranted due to their particular toxicity and potentially significant persistence. Other likely breakdown products such as thiodiglycol from HD, and methylphosphonic acid (MPA) from the G-agents and VX, do not pose a significant health risk. However, due to their persistence in the environment, they may be useful indicators of historical chemical warfare agent presence.

**11.3.4** It is unlikely that the chemical agents addressed in this document will contaminate ground water. Site-specific evaluations are recommended to identify those circumstances where potential ground-water contamination should be evaluated. It is also unlikely that these agents would contaminate a drinking water source. Site-specific assessment should be conducted only for those circumstances where contamination of a drinking water source is a realistic concern.

**11.3.5** Other applications of these models may be an appropriate mechanism to assess other scenarios where there is potential for long-term or repeated exposures (such as for waste management or when assessing nonpervious contaminated surfaces). For these potential applications of chronic risk assessment models, common generic assumptions do not currently exist. Evaluating risks in these scenarios is the subject of potential future initiatives.

#### **11.4 KEY UNCERTAINTIES ASSOCIATED WITH THE CHEMICAL WARFARE AGENT HBESLs**

Uncertainties within the assessment process can result in either an overconservative (e.g., the HBESL concentration may actually be lower than a level that will protect public health) or underconservative (e.g., the HBESL may not be low enough to ensure protection of public health). Several areas of uncertainty were identified during the evaluation of these screening level methodologies. This is typical of input parameters for which there is limited information or which represent general theoretical scenarios as opposed to a specific site. Even for parameters with sufficient data, it is sometimes necessary to use professional judgement based on experience to determine which are best for a particular situation. In this evaluation, the uncertainties are not necessarily specific to the calculation of screening levels for *chemical warfare agents*, but also span a variety of data gaps and generalizations that are also imparted to screening levels that are established for commercial chemical compounds. This section summarizes some of the major data gaps - both general and chemical agent specific.

The uncertainties begin with the actual models (or mathematical algorithms) currently used in the environmental risk assessment process; in particular on the issue of how accurately such models describe the process of exposure from a source. The other uncertainties are associated with the assumptions that go into these models. Overall, the types of uncertainty may be broken down into three general categories: 1) model uncertainty, 2) exposure uncertainty, and 3) toxicity data uncertainty.

Examples of model uncertainties include whether or not all pathways should result in an additive exposure or whether pathways appropriately represent real-world processes. Exposure parameter uncertainties include the variability or unknown aspects of exposure. Parameters such as exposure frequency and duration are primary examples of parameters which may have a significant impact on the resulting calculated values, but for which it is inherently difficult to determine how accurately the assumed value represents a true occurrence.

The chronic toxicity values are extremely important to the overall estimation of risk or calculated screening level value. Several uncertainties such as human variability, extrapolation from animal data, and extrapolation of acute or subchronic data to estimate a chronic threshold are just a few examples of the many assumptions that must be accounted for in the development of the values used in the risk assessment model. Overall, the balance of uncertainty in the calculation is designed to 'err' on the side of conservatism.

Ascertaining the degree and overall effect/impact of the uncertainty associated with a calculated screening level cannot be done quantitatively. However, a qualitative evaluation provides essential information to consider when using such screening levels as a decision-tool. Various uncertainties associated with the models themselves, as well as with the individual input parameter assumptions, have been described in detail throughout this document. Additional uncertainties associated with the application of the models to less common scenarios are summarized in the individual unique scenario example appendices. Some of the key uncertainties and their effects on the HBESLs associated with the scenarios described in the main text of this document are summarized in Table 11-1.

<b>Table 11-1. Key Areas of Uncertainty and Effect on Conservatism of HBESL</b>		
Type of Uncertainty	Discussion	Effect On Conservatism of HBESL <sup>a</sup>
Single Pathway Models - RBCs, SSLs	For the nerve agents (GA, GB, GD, and VX) the use of these models may underestimate risk by only addressing single exposure pathways (assuming cumulative effects even through different routes of exposure)	
	For the vesicants (HD and Lewisite), the effects may not be the same if introduced through different routes of exposures; may be most appropriate	
Multipathway Model - PRG	For the nerve agents (GA, GB, GD, and VX) the use of this model seems the most justifiable in that it sums the total effects on the body (assuming same effects even through different routes of exposure)	
	For the vesicants (HD and Lewisite), the effects may not be the same if introduced through different routes of exposures; adding all pathways may be slightly overconservative	



<b>Table 11-1. Key Areas of Uncertainty and Effect on Conservatism of HBESL</b>		
Environmental degradation	Natural degradation processes such as photo degradation and environmental half-life were not included in the concepts of the chronic risk model - rather a continued long-term exposure to these concentrations is assumed even though this situation may not be reasonably expected under most environmental conditions.	
Toxicity endpoints	Noncancer chemical agent RfDs; peer-reviewed chronic life-time dose estimates currently under review by NRC, COT but approved by DA OTSG for interim use - believed to be conservative estimates	
	Cancer slope factor for HD; Recent study by Gaylor (1998) indicated that the CSF for HD ranges from 1.6 to 9.5 mg/kg/day <sup>-1</sup> . To be conservative, USEPA's proposed value of 95 mg/kg/day <sup>-1</sup> was also included to derive a geometric mean for HD CSF.	
Organic carbon partition coefficient ( $K_{oc}$ )	This parameter was estimated by using a regression relationship based on each chemical agent's octanol-water partition coefficient ( $K_{ow}$ ). Actual experimental values may be different for each chemical agent.	
Soil water partition coefficient ( $K_d$ )	The $K_d$ was estimated from the chemical's $K_{oc}$ and by assuming a soil organic carbon content. Actual site-specific value may differ depending on the organic carbon content.	
Exposure duration (ED)	USEPA default exposure durations were used for each of the exposure scenarios. The length of time an individual resides at a location may vary; however, the defaults are conservative for the specified scenarios in the main document	
Skin surface area (SA)	Default SAs were used and assumed to be reasonably conservative for the given scenarios. However, this parameter may be significantly impacted by individual variation, clothing, temporal, and seasonal factors.	
Exposure frequency (EF)	USEPA default values were used for the scenarios presented in the main portion of this document. The EF may vary between individuals; however, the defaults are conservative for the specified scenarios in the main document.	
Soil-to-skin adherence factor (AF)	Site-specific soil data may indicate that this parameter is higher or lower than the USEPA default.	

<b>Table 11-1. Key Areas of Uncertainty and Effect on Conservatism of HBESL</b>		
Dermal absorption factor	An organic carbon content of 2% was assumed for the purpose of estimating dermal absorption from the soil. Actual organic carbon content can vary from site to site.	
	The absorption factor is assumed to be constant over the total period of exposure (8 and 12 hours).	
GI absorption factor	Dermal toxicity values were extrapolated from each chemical agent's oral toxicity value. Due to lack of chemical-specific GI absorption factors, a default GI of 100% was assumed. Actual GI absorption factors may be lower.	

- <sup>a</sup> : uncertainty results in an overconservative HBESL  
: uncertainty results in an underconservative HBESL  
: effect on conservatism of HBESL may vary

## 11.5 RECOMMENDATIONS

The Table below lists HBESL values for two common generic scenarios using three current EPA chronic risk assessment methods, common default and chemical-specific parameters. The information in this document can be used to help stakeholders determine if screening levels can be used, and if so, what models and parameters best fit site-specific needs. The HBESLs can be used as action/no-action determinants ('action' meaning to perform site-specific health risk assessment; apply management controls; treat/remediate; or a combination of these) when assessing the potential for chronic health effects to exposed populations so long as the following conditions are met:

**11.5.1** *Levels of risk are acceptable to the situation (see Section 1.3.2).* This can only be assessed through negotiation with applicable regulators and other stakeholders.

**11.5.2** *Assumptions made in these scenarios are at least equally conservative, if not more conservative, than site-specific values.* For example, if the exposure to persons in a hypothetical industrial scenario is anticipated to be less than 100 days/yr, the HBESL exposure frequency assumption of 250 days/yr is more conservative; therefore allowing for a conservatively 'safe' screening decision.

**11.5.3** *Substance concentrations and exposure assumptions are not expected to be acutely toxic (see Section 1.3.8).* For scenarios involving limited exposure duration and frequency values, these models should be used only with extreme caution. In certain cases the application of these chronic risk assessment models may be inappropriate and acute toxicity to short-term exposures should be evaluated separately.

**11.5.4** *A single chemical is of concern (see Section 1.3.9).*

**11.5.5** *Ground-water contamination is not considered to be a concern (see Appendix E).*

**11.5.6** *Risk to ecological receptors is not expected (see Section 1.3.10).* HBESLs listed in this document do NOT address ecological risk, and may not be sufficiently conservative to protect all ecological receptors at all sites.

Table 11-2. Range of Estimated HBESL Values for Chemical Warfare Agents						
	Residential soil (mg/kg)			Industrial soil (mg/kg)		
	RBCs	PRGs	SSLs	RBCs	PRGs	SSLs
<b>HD</b>	0.55	0.01 <sup>a</sup>	0.016	14	0.3 <sup>a</sup>	NA
<b>Lewisite<sup>c</sup></b>	7.8	0.3	7.8	(7.8) <sup>d</sup>	3.7	NA
<b>GA</b>	3.1	2.8	0.8	82	68	NA
<b>GB</b>	1.6	1.3	0.5	41	32	NA
<b>GD</b>	0.31	0.22	0.18	8.2	5.2	NA
<b>VX<sup>b</sup></b>	0.047	0.042	0.047	1.2	1.1	NA

<sup>a</sup> Cancer-based; residential target risk level of  $10^{-5}$ , industrial target risk level of  $10^{-4}$

<sup>b</sup> Assessment should include EA-2192, a particularly toxic and relatively persistent breakdown component of VX. Due to similar toxicity, the HBESLs derived for VX can be used for EA-2192.

<sup>c</sup> Assessment should include CVA/Lewisite oxide & arsenic, persistent breakdown products of Lewisite. USEPA screening levels for inorganic arsenic should be consulted. HBESLs for Lewisite can be used for CVA and Lewisite oxide.

<sup>d</sup> RBC value derived for the commercial/industrial scenario was potentially above acute toxicity levels, therefore the upper bound value of the residential scenario is suggested as a substitute.

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## GLOSSARY

ABS<sub>derm</sub>: Dermal Absorption Factor

ABS<sub>gi</sub>: Gastrointestinal Absorption Factor

Absorbed Dose: The amount of a substance penetrating the exchange boundaries of an organism after contact. Absorbed dose is calculated from the intake and the absorption efficiency. It usually is expressed as mass of a substance absorbed into the body per unit body weight per unit time (e.g., mg/kg-day).

Absorption: The penetration of a substance into or through another substance or medium. The uptake and entry of a substance through intact skin, eyes, gastrointestinal tract or lungs (i.e., ingestion or once the substance has entered the lungs).

Acetylcholinesterase: A member of the cholinesterase group of enzymes that is naturally present at nerve endings and in red blood cells and which normally breaks down acetylcholine into acetic acid and choline; an enzyme that is inhibited by nerve agents.

Adsorption: The adhesion of a substance to the surface of another solid or liquid (not to be confused with absorption).

Adverse Effect Level (AEL): An exposure level at which there are statistically or biologically significant increases in frequency or severity of deleterious effects between the exposed population and its appropriate control group.

AF<sub>a</sub>: Soil-to-Skin Adherence Factor for adult

AF<sub>c</sub>: Soil-to-Skin Adherence Factor for child

Agent GA: The chemical ethyl N,N-dimethylphosphoramidocyanidate, Chemical Abstracts Service (CAS) registry number 77-81-6, in pure form and in the various impure forms found in military storage as well as in military industrial, depot, or laboratory operations (synonym = Tabun); a nerve agent with chemical formula C<sub>5</sub>H<sub>11</sub>N<sub>2</sub>O<sub>2</sub>P.

Agent GB: The chemical isopropyl methylphosphonofluoridate, CAS number 107-44-8, in pure form and in the various impure forms found in military storage as well as in military industrial, depot, or laboratory operations (synonym = Sarin); a nerve agent with chemical formula C<sub>4</sub>H<sub>10</sub>FO<sub>2</sub>P.

Agent GD: The chemical pinacolyl methyl phosphonofluoridate, CAS number 96-64-0, in pure form and in the various impure forms found in military storage as well as in military industrial, depot, or laboratory operations (synonym = Soman); a nerve agent with chemical formula C<sub>7</sub>H<sub>16</sub>FO<sub>2</sub>P.

Agent H: Levinstein mustard; a mixture of 70 percent bis(2-chloroethyl) sulfide, CAS # 505-60-2, and 30 percent sulfur impurities produced by the Levinstein process. Agent H is a blister agent and is unstable.

Agent HD: Distilled mustard or bis(2-chloroethyl) sulfide, CAS registry number 505-60-2. Distilled

mustard (HD) is mustard (H) that has been purified by washing and vacuum distillation to reduce sulfur impurities; a blister agent with chemical formula  $C_4H_8Cl_2S$ .

Agent HT: A plant-run mixture containing about 60 percent HD and <40 percent agent T plus a variety of sulfur contaminants and impurities. Agent T is bis [2-(2-chloroethylthio)ethyl]ether, CAS registry number 63918-89-8, and is a sulfur, oxygen and chlorine compound similar in structure to HD (Agent T has chemical formula  $C_8H_{16}Cl_2OS_2$ ). Agent HT is a blister agent with a lower freezing point than agent HD.

Agent L, or Lewisite: 2-chlorovinyl dichloroarsine, CAS registry number 541-25-3; agent L is a blister agent with the chemical formula  $C_2H_2AsCl_3$ .

Agent VX: The chemical O-ethyl S-(2-diisopropylaminoethyl)methylphosphonothioate, CAS registry number 50782-69-9, in pure form and in the various impure forms that may be found in military storage as well as in military industrial, depot, or laboratory operations. Agent VX is a nerve agent.

AIHC: American Industrial Health Council

$AT_c$ : Averaging time used in HBESL calculations for carcinogens

$AT_n$ : Averaging time used in HBESL calculations for noncarcinogens; residential, industrial

Blister Agent: A compound (such as sulfur mustard) that produces local irritation and damage to the skin, eyes and respiratory tract, and mucous membranes; injury may progress in severity to fluid-filled blisters (vesicles) on skin, depending on degree of exposure to liquid or vapor.

$BW_a$ : Body weight for adult

$BW_c$ : Body weight for child

$BW_t$ : Body weight for adolescent trespasser

Carcinogen: A substance or condition known to induce neoplastic change (malignancies) in experimental animals and/or man. Four types of response are generally accepted as evidence of neoplasm induction or increased carcinogenic risk:

- a. An increase in incidence of the tumor types that occur vs those found in controls.
- b. The development of tumors earlier than controls.
- c. The occurrence of tumor types not observed in controls.
- d. An increased multiplicity of tumors.

Carcinogenicity: Refers to the potential for development of cancer in a living individual. A cancer is a malignant tumor resulting from a change in the normal growth and development of cells. Cancer tumors have the tendency to invade surrounding tissue and spread to other sites in the body.

CAS: Chemical Abstracts Service

CDC: Centers for Disease Control and Prevention, U.S. Department of Health and Human Services, Atlanta,

## GA

CERCLA: The Comprehensive Environmental Response, Compensation, and Liability Act of 1980; also known as "Superfund".

ChE: abbreviation for cholinesterase; see definition for "cholinesterase" below.

Chemical of Potential Concern (COPC): Chemicals that are potentially site-related and whose data are of sufficient quality for use in the quantitative risk assessment.

Chemical Warfare Agent: A chemical substance intended for use in military operations to kill, seriously injure, or incapacitate people through its physiological effects. Included are blood, nerve, choking, blister, and incapacitating agents. Excluded are riot control agents, chemical herbicides, and smoke and flame materials.

Choline: One of the products from the hydrolysis of acetylcholine;  $C_5H_{15}O_2N$ .

Cholinesterase (ChE): A naturally occurring enzyme that catalyzes the hydrolysis of the naturally occurring neurotransmitter acetylcholine to choline (a vitamin) and an anion. Acetylcholinesterase is such an enzyme.

Chronic Reference Dose (RfD): An estimate (with uncertainty spanning perhaps an order of magnitude or greater) of a daily exposure level (usually in units of mg of chemical /kg body weight/day) for the human population, including sensitive subpopulations, that is likely to be without an appreciable risk of deleterious effects during a lifetime. Chronic RfDs are specifically developed to be protective for long-term exposure to a compound (as a Superfund program guideline, seven years to lifetime).

CSEPP: Chemical Stockpile Emergency Preparedness Program

COT: National Research Council Committee On Toxicology

CSF: Cancer Slope Factor; see definition for Slope Factor

Ct: concentration (often in  $mg/m^3$ ) multiplied by the time period (usually in min) of exposure duration; a measure of cumulative exposure. For nerve agents, acute Cts appear to be valid only for short (approx. 10 min) periods; thus, Ct does not equal k for exposure periods greater than approx. 30-50 min. For example, a 2-minute exposure to a concentration of 100  $mg/m^3$  [ $Ct = 200 \text{ mg-min}/m^3$  (milligram-minutes per cubic meter)], does NOT necessarily produce the same toxicological effects as a 50-minute exposure to a concentration of 4  $mg/m^3$  ( $Ct = 200 \text{ mg-min}/m^3$ ).

CVA: 2-Chlorovinyl arsonic acid

Dermal Exposure: Exposure to or by absorption through the skin.

DHHS: U.S. Department of Health and Human Services

Detection Limit (DL): The lowest amount of a compound of interest that can be distinguished from the normal "noise" of an analytical instrument or method; has been defined as 3.3 times the standard deviation of the response and slope of the calibration curve (see Krull and Swartz 1998)

Developmental Reference Dose ( $RfD_{dt}$ ): an estimate (with uncertainty spanning perhaps an order of magnitude or greater) of an exposure level for the human population, including sensitive subpopulations, that is likely to be without an appreciable risk of developmental effects. Developmental  $RfDs$  are used to evaluate the effects of a single exposure event.

DAF: Dilution Attenuation Factor

Dosage: The amount of substance administered (or received) per unit body weight or surface area (as mg/kg or mg/cm<sup>2</sup>).

Dose: The amount of agent or energy that is absorbed by the body; the amount of substance, radiation, or energy absorbed in a unit volume, an organ, or an individual (as mg/animal).

EA2192: S-(Diisopropylaminoethyl) methylphosphonothioate; a VX degradation product

$ED_c$ : Exposure duration for child in residential scenario (for soil contamination)

$ED_i$ : Exposure duration for industrial scenario

$ED_r$ : Exposure duration for residential scenario (for water contaminants)

$ED_t$ : Exposure duration for adolescent trespasser

$EF_i$ : Exposure frequency for industrial scenario

$EF_r$ : Exposure frequency for residential scenario

ERAP: Environmental Risk Assessment Program; part of the Strategic Environmental Research Development Program.

Exposure: Contact of an organism with a chemical or physical agent. Exposure is quantified as the amount of the agent available at the exchange boundaries of the organism (e.g., skin, lungs, gut) and available for absorption.

Exposure Assessment: The determination or estimation (qualitative or quantitative) of the magnitude, frequency, duration, and route of exposure.

Exposure event: An incident of contact with a chemical or physical agent. An exposure event can be defined by time (e.g., day, hour) or by the incident (e.g., eating a single meal of contaminated fish).

Exposure Pathway: The course a chemical or physical agent takes from a source to an exposed organism. An exposure pathway describes a unique mechanism by which an individual or population is exposed to chemicals or physical agents at or originating from a site. Each exposure pathway includes a source or release from a source, an exposure, an exposure point, and an exposure route. If the exposure point differs from the source, a transport/exposure medium (e.g. air) or media (in case of inter-media transfer) also is included.

FUDS: Formerly Used Defense Site

H: Henry's Law Constant; the ratio of a chemical's volatility to its water solubility. Another and separate



definition is Levinstein mustard, or agent H.

HD: Distilled Mustard – see Agent HD

HBESL: Health-Based Environmental Screening Level

HEAST: Superfund Health Effects Assessment Summary Tables

Hydrolyzed: Refers to a compound which has undergone chemical reaction with liquid water or water vapor; hydrolysis is the reaction of a particular compound (such as a chemical warfare agent) with water to form new chemical compounds ("reaction products") which are degradation products of the parent compound.

IDLH: Immediately Dangerous to Life or Health; a concept originally developed by the National Institute for Occupational Safety and Health (NIOSH) in the 1970s for use in selecting respiratory protection; the maximum concentration from which, in the event of respirator failure, one could escape within 30 minutes without a respirator and without experiencing any irreversible health effects or escape-impairing effects. IDLH values are not intended for establishing permissible exposure limits. IDLH values for industrial compounds are published annually in the NIOSH *Pocket Guide to Chemical Hazards*.

IFA<sub>adj</sub>: Inhalation factor, age adjusted

IFS<sub>adj</sub>: Soil ingestion factor, age adjusted

InhF<sub>adj</sub>: Inhalation factor, age adjusted

Intake: A measure of exposure expressed as the mass of a substance in contact with the exchange boundary per unit body weight per unit time (e.g., mg chemical/kg-day). Also termed the normalized exposure rate; equivalent to administered dose.

IRA<sub>a</sub>: Inhalation rate for adult

IRA<sub>c</sub>: Inhalation rate for child

IRA<sub>i</sub>: Inhalation rate for industrial scenario

IRIS: The USEPA Integrated Risk Information System; a USEPA database containing verified RfDs, slope factors and up-to-date health risk and USEPA regulatory information for numerous chemicals. IRIS is USEPA's preferred source for Superfund toxicity information.

IRS<sub>a</sub>: Soil ingestion for adult, residential scenario

IRS<sub>c</sub>: Soil ingestion for child

IRS<sub>i</sub>: Soil ingestion for adult, industrial scenario

Lowest-Effect Level (LEL): The lowest exposure level at which there are statistically or biologically significant increases in frequency or severity of effects between the exposed population and its appropriate control group. Not necessarily an **adverse** effect level.

Lowest-Observed Adverse Effect Level (LOAEL): In dose-response experiments, the lowest exposure level at which there are statistically or biologically significant increases in frequency or severity of adverse effects between the exposed population and its appropriate control group.

MCL: Maximum Contaminant Level

MCLG: Maximum Contaminant Level Guideline

MEL: Minimum Effect Level for acute toxicity; lowest exposure level at which there is detectable response.

Mustard: usually, sulfur mustard agent; the chemical bis(2-chloroethyl) sulfide, CAS registry number 505-60-2, in pure form and in the various impure formulations that may be found in chemical munitions as well as CW field, industrial, or laboratory operations; a vesicant agent. These formulations include Levinstein mustard (H), distilled mustard (HD), and closely related preparations. This definition does not apply to nitrogen mustards.

NAPL: Non Aqueous-Phase Liquid

National Contingency Plan (NCP): The “National Oil and Hazardous Substances Pollution Contingency Plan” prepared by the USEPA to implement comprehensive environmental response, compensation and liability under CERCLA and the Clean Water Act; directs responsibility and procedures for cleanup of hazardous material spills. The regulations are codified at 40 CFR 300, et seq.

Nerve Agent: One of the several organic esters of phosphoric acid used as chemical warfare nerve agents because of their extreme toxicity (Tabun, GA; Sarin, GB; Soman, GD; GF, and VX). All are potent inhibitors of the enzyme, acetylcholinesterase, which is responsible for the degradation of the neurotransmitter, acetylcholine. Symptoms result from excess accumulation of acetylcholine in neuronal synapses or myoneural junctions. Nerve agents are readily absorbed by inhalation and/or through intact skin.

NIOSH: The National Institute for Occupational Safety and Health of the U.S. Department of Health and Human Services

NRC: the National Research Council

Non-detects (NDs): Chemicals that are not detected in a particular sample at concentrations below a certain limit, usually the detection limit for the chemical in that sample. Non-detects may be indicated by a “U” data qualifier.

No-Observed Adverse Effects Level (NOAEL): In dose-response experiments, an exposure level at which there are no statistically or biologically significant increases in the frequency or severity of adverse effects (to tissue, cells, organs, etc.) between the exposed population and its appropriate control (some effects may be produced at this level, but they are not considered as adverse, nor precursors to specific adverse effects). The NOAEL is the highest exposure level without adverse effect.

No-Observed Effects Level (NOEL): An exposure level at which there are no statistically or biologically significant increases in the frequency or severity of any effect (to tissue, cells, organs, etc.) between the exposed population and its appropriate control.

ORNL: Oak Ridge National Laboratories

OSHA: Occupational Safety and Health Administration

OSWER: USEPA Office of Solid Waste and Emergency Response

OTSG: Office of The (Army) Surgeon General

PEF: Particulate Emission Factor

Percutaneous Exposure: The absorption of a contaminant through the unbroken skin.

PPE: Personal Protective Equipment

ppm: Parts per million

PRG: USEPA Region IX Preliminary Remediation Goal model (see USEPA 1996a)

Quantitation Limit (QL): The lowest level at which a chemical can be accurately and reproducibly detected. Various definitions; one recent definition is 10 times the standard deviation of the response and slope of the calibration curve (Krull and Swartz, 1998); definition varies for different chemicals and different samples.

RAGS: Risk Assessment Guidance for Superfund; the document *Risk Assessment Guidance for Superfund, volume 1: Human Health Evaluation Manual*, Parts A and B. EPA/540/1-89/002 and Pub. # 9285.7-01B of the USEPA Office of Emergency Response (1989).

RASH: Rapid Screening of Hazard relative potency approach for the assessment of toxicity; documented in Jones et al 1985 and Jones et al 1988

Reference Concentration (RfC): An estimate (with uncertainty spanning perhaps an order of magnitude) of a daily inhalation exposure to the human population (including sensitive subgroups) that is likely to be without appreciable risk of deleterious effects during a lifetime.

Reference Dose (RfD): the USEPA's preferred toxicity value (in units of mg chemical/kg body weight/day) for evaluating noncarcinogenic effects resulting from exposure at Superfund sites. See specific entries for chronic RfD, subchronic RfD, and developmental RfD. The acronym RfD, when used without other modifiers, either refers generically to all types of RfDs or specifically to chronic RfDs; it never refers specifically to subchronic or developmental RfDs.

Remedial Actions: Actions taken to restore a contaminated site to its pre-contaminated condition. In contrast to removal actions, these are longer-term actions, including cleanup, treatment, and neutralization of contamination and access control or permanent relocation of residents, if necessary. Remedial actions are coordinated by the remedial project manager. U.S. Department of the Army Pamphlet (DA PAM) 50-6, *Chemical Accident or Incident Response and Assistance (CAIRA) Operations*, treats remedial actions as taking place in a "non-emergency atmosphere," and describes the goal as returning the chemical accident or incident site to "technically achievable and acceptable conditions."

RBC: USEPA Region III Risk-Based Concentration model

RME: Reasonable maximum exposure; the highest exposure that is reasonably expected to occur at a site

SA<sub>a</sub>: Exposed skin surface for adult

SA<sub>c</sub>: Exposed skin surface for child

Sarin: Isopropyl methylphosphonofluoridate, CAS number 107-44-8; it is a nonpersistent organophosphate nerve agent also known as Agent GB. Its chemical formula is C<sub>4</sub>H<sub>10</sub>FO<sub>2</sub>P.

SERDP: Strategic Environmental Research Development Program

SFS<sub>adj</sub>: Soil contact factor, age adjusted

Slope Factor: A plausible upper-bound estimate of the probability of a response per unit intake of a chemical over a lifetime. The slope factor is used to estimate an upper-bound probability of an individual developing cancer as a result of a lifetime of exposure to a particular level of a potential carcinogen.

Soman: Pinacolyl methyl phosphonofluoridate, CAS number 96-64-0; nerve agent GD. Its chemical formula is (CH<sub>3</sub>)<sub>3</sub>CCH(CH<sub>3</sub>)OPF(O)CH<sub>3</sub>.

SSL: USEPA-OSWER Soil Screening Level model

STEL: Short-Term Exposure Limit; see also definition for TLV-STEL

Subchronic reference dose (RfD<sub>s</sub>): An estimate (with uncertainty spanning perhaps an order of magnitude or greater) of a daily exposure level for the human population, including sensitive subpopulations, that is likely to be without an appreciable risk of deleterious effects during a portion of a lifetime (as a Superfund program guideline, two weeks to seven years).

Sulfur Mustard: A blister agent also known as Agent H (or HD for distilled mustard); bis(2-chloroethyl) sulfide, CAS number 505-60-2. The chemical formula is C<sub>4</sub>H<sub>8</sub>Cl<sub>2</sub>S.

Tabun: Ethyl N,N-dimethylphosphoramidocyanidate, CAS number 77-81-6. A non-persistent organophosphate nerve agent also known as Agent GA. Its chemical formula is C<sub>5</sub>H<sub>11</sub>N<sub>2</sub>O<sub>2</sub>P.

Threshold Limit Value (TLV<sup>®</sup>): TLV<sup>®</sup> is a registered trademark of the American Conference of Governmental Industrial Hygienists, Cincinnati, Ohio. A value that refers to airborne concentrations of substances and represents conditions under which it is believed nearly all workers may be repeatedly exposed day after day, without adverse health effects. A table of these values and accompanying precautions is published annually by the ACGIH. Use of trademarked name does not imply endorsement by the U.S. Army but is intended only to assist in identification of a specific product.

Threshold Limit Value Categories:

a. Threshold Limit Value-Time-Weighted Average (TLV-TWA). The time-weighted average concentration for a normal 8-hour workday and a 40-hour workweek, to which nearly all workers may be repeatedly exposed, day after day, without adverse effect.

b. Threshold Limit Value-Short-Term Exposure Limit (TLV-STEL). The concentration to which workers can be exposed continuously for a short period of time without suffering from (1) irritation,

(2) chronic or irreversible tissue damage, or (3) narcosis of sufficient degree to increase the likelihood of accidental injury, impair self-rescue, or materially reduce work efficiency, provided that the daily TLV-TWA is not exceeded. The STEL is not a separate independent exposure limit; rather, it supplements the time-weighted average (TWA) limit where there are recognized acute effects from a substance whose toxic effects are primarily of a chronic nature. Exposures up to the STEL should not be longer than 15 minutes and should not occur more than four times per day, with a period of at least 60 min between successive exposures.

c. Threshold Limit Value--Ceiling (TLV-C). The concentration that should not be exceeded during any part of the working exposure.

**Time-Weighted Average (TWA) Concentration:** The concentration of airborne material that has been weighted for the time duration, usually eight hours. A sufficient number of samples are needed to determine a TWA concentration throughout a complete cycle of operations or through the work shift.

**Time-Weighted Average Exposure:** An average over a given (working) period of an individual's exposure, as determined by sampling at given times during the period.

**Toxicity:** The capacity of a chemical to act as a poison in producing harmful effects on living organisms; the nature, degree, and extent of undesirable effects.

**TR:** target excess individual lifetime cancer risk (unitless)

**Uncertainty Factor (UF):** One of several adjustment factors used in operationally deriving a RfD from experimental data and representing a specific area of uncertainty inherent in the extrapolation from available data. Each UF value is often 10, although values <10 can also be used. UFs are intended to account for:

- a. Human to sensitive human; intended to protect sensitive subpopulations.
- b. Animal to human; extrapolating from animal data to the case of humans.
- c. Subchronic to chronic; extrapolating from a subchronic study to derive a chronic RfD.
- d. LOAEL to NOAEL; when a suitable NOAEL is not available and a LOAEL is used instead.
- e. Incomplete to complete database; when available data do not adequately address all possible adverse outcomes in humans.

**USACHPPM:** U.S. Army Center for Health Promotion and Preventive Medicine

**USEPA:** U.S. Environmental Protection Agency

**Vesicant:** Causing blisters or vesicles. Sulfur mustard agent (HD) and Lewisite (L) are both vesicant agents.

**VF<sub>s</sub>:** Volatilization Factor for soil

**VF<sub>w</sub>:** Volatilization Factor for tapwater.

**VLEACH:** a one-dimensional finite difference vadose zone leaching model. The model estimates the impact on underlying ground water of the mobilization and migration of sorbed organic pollutants located in

the vadose zone.

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## APPENDIX A

### DERIVATION OF CHEMICAL PARAMETERS

#### A.1 HENRY'S LAW CONSTANT

This constant is a ratio of the volatility of a chemical to its water solubility, and thus is a measure of the tendency of a chemical to volatilize from water. Henry's Law Constants can be determined experimentally or estimated from the vapor pressure and water solubility of the chemical.

$$H = \frac{V}{S} \quad (\text{A-1})$$

where:

V = vapor pressure (in atm)

S = water solubility (in mol/m<sup>3</sup>)

or

$$H = H^* \times R \times T \quad (\text{A-2})$$

where:

H\* = ratio of the volatility (in mg/m<sup>3</sup>) and water solubility (in mg/m<sup>3</sup>)

R = gas constant (8.2 x 10<sup>-5</sup> atm·m<sup>3</sup>/mol·K)

T = temperature in K (20°C = 293.15°K)

Henry's Law Constants for the chemical warfare agents were derived using both Equation A-1 and Equation A-2. The derived values are presented in Table A-1.

#### A.2 DIFFUSION COEFFICIENTS

##### A.2.1 Diffusivity in Air

For the diffusion of a chemical in air the following formula is recommended (USEPA, 1994a):

$$Di = 0.0067T^{1.5} (0.034 + M^{-1})^{0.5} M^{-0.17} [(M/2.5d)^{0.33} + 1.81]^{-2} \quad (\text{A-3})$$

where:

T = Absolute temperature (degrees Kelvin)

M = Molecular weight (g/g mol)

d = Density of liquid chemical (g/cm<sup>3</sup>)

Table A-1. Vapor pressure, Solubility and Henry's Law Constants for Chemical Warfare Agents									
Chemical (mol. wt)	Vapor pressure (mm Hg)	Vapor Pressure (atm)	Volatility (mg/m <sup>3</sup> )	Solubility (g/100 g)	Solubility (mg/m <sup>3</sup> )	Solubility (mol/m <sup>3</sup> )	Henry's Law Constant (atm·m <sup>3</sup> /mol)		
							Derived from Equation A-1	Derived from Equation A-2	Literature Value <sup>a</sup>
HD <sup>b</sup> (159.08)	0.11 <sup>c</sup>	1.4 x 10 <sup>-4</sup>	920 <sup>c</sup>	0.092 <sup>d</sup>	9.2 x 10 <sup>5</sup>	5.8 <sup>c</sup>	2.4 x 10 <sup>-5</sup>	2.4 x 10 <sup>-5</sup>	2.1 x 10 <sup>-5</sup>
Lewisite (207.32)	0.58 <sup>c</sup>	7.6 x 10 <sup>-4</sup>	6500 <sup>c</sup>	0.05 <sup>f,g</sup>	5 x 10 <sup>5</sup>	2.4	NA <sup>g</sup>	NA <sup>g</sup>	-
GA (162.1)	0.07 <sup>c</sup>	9.2 x 10 <sup>-5</sup>	610 <sup>c</sup>	9.8 <sup>c</sup>	9.8 x 10 <sup>7</sup>	604.6	1.5 x 10 <sup>-7</sup>	1.5 x 10 <sup>-7</sup>	-
GB (140.1)	2.9 <sup>c</sup>	3.8 x 10 <sup>-3</sup>	22000 <sup>c</sup>	miscible	miscible	miscible	-	-	5.4 x 10 <sup>-7</sup>
GD (182.2)	0.40 <sup>c</sup>	5 x 10 <sup>-4</sup>	3900 <sup>c</sup>	2.1 <sup>e</sup>	2.1 x 10 <sup>7</sup>	115.3	4.3 x 10 <sup>-6</sup>	4.5 x 10 <sup>-6</sup>	-
VX (267.4)	0.0007 <sup>c</sup>	9 x 10 <sup>-7</sup>	10.5 <sup>c</sup>	3 <sup>c</sup>	3 x 10 <sup>7</sup>	112.2	8.0 x 10 <sup>-9</sup>	8.4 x 10 <sup>-9</sup>	3.5 x 10 <sup>-9</sup>

**Source:** Vapor pressure, volatility, and solubility data from DA, 1974

<sup>a</sup> Small, 1984

<sup>b</sup> Volatility and solubility data not for same temperature.

<sup>c</sup> At 25°C

<sup>d</sup> At 22°C

<sup>e</sup> At 20°C

<sup>f</sup> MacNaughton and Brewer, 1994

<sup>g</sup> Lewisite hydrolyzes so rapidly that measurements of solubility and calculation of H are not meaningful (Rosenblatt et al., 1975)



**A.2.1.1 Sulfur Mustard.** The molecular weight of HD is 159.02 and the liquid density is 1.27 g/ml. At a temperature of 300°K, the air diffusivity coefficient for HD is:

$$Di = 0.0067 \times 300^{1.5} (0.034 + 159.02^{-1})^{0.5} 159.02^{-0.17} [(159.02/(2.5 \times 1.27))^{0.33} + 1.81]^{-2} \quad (\text{A-4})$$

$$Di = 0.099$$

**A.2.1.2 Lewisite.** The molecular weight of Lewisite is 207.32 and the liquid density is 1.88 g/ml. At a temperature of 300°K, the air diffusivity coefficient for Lewisite is:

$$Di = 0.0067 \times 300^{1.5} (0.034 + 207.32^{-1})^{0.5} 207.32^{-0.17} [(207.32/(2.5 \times 1.88))^{0.33} + 1.81]^{-2} \quad (\text{A-5})$$

$$Di = 0.099$$

**A.2.1.4 Agent GA.** The molecular weight of GA is 162.1 and the liquid density is 1.09 g/ml. At a temperature of 300°K, the air diffusivity coefficient for GA is:

$$Di = 0.0067 \times 300^{1.5} (0.034 + 162.1^{-1})^{0.5} 162.1^{-0.17} [(162.1/(2.5 \times 1.09))^{0.33} + 1.81]^{-2} \quad (\text{A-6})$$

$$Di = 0.092$$

**A.2.1.3 Agent GB.** The molecular weight of GB is 140.1 and the liquid density is 1.09 g/ml. At a temperature of 300°K, the air diffusivity coefficient for GB is:

$$Di = 0.0067 \times 300^{1.5} (0.034 + 140.1^{-1})^{0.5} 140.1^{-0.17} [(140.1/(2.5 \times 1.09))^{0.33} + 1.81]^{-2} \quad (\text{A-7})$$

$$Di = 0.101$$

**A.2.1.5 Agent GD.** The molecular weight of GD is 182.2 and the liquid density is 1.02 g/ml. At a temperature of 300°K, the air diffusivity coefficient for GD is:

$$Di = 0.0067 \times 300^{1.5} (0.034 + 182.2^{-1})^{0.5} 182.2^{-0.17} [(182.2/(2.5 \times 1.02))^{0.33} + 1.81]^{-2} \quad (\text{A-8})$$

$$Di = 0.082$$

**A.2.1.6 Agent VX.** The molecular weight of VX is 267.37 and the liquid density is 1.0083 g/mL. At a temperature of 300°K, the air diffusivity coefficient for VX is:

$$Di = 0.0067 \times 300^{1.5} (0.034 + 267.37^{-1})^{0.5} 267.37^{-0.17} [(267.37/(2.5 \times 1.0083))^{0.33} + 1.81]^{-2} \quad (\text{A-9})$$

$$Di = 0.062$$

## A.2.2 Diffusivity in Water

For the diffusion of a chemical in water the following formula is recommended (USEPA, 1994a):

$$D_w = 1.518 (10^{-4}) V_{cm}^{-0.6} \quad (\text{A-10})$$

where:

$D_w$	=	Diffusion coefficient in water
$V_{cm}$	=	Molar volume (M/d)
$M$	=	Molecular weight of chemical
$d$	=	Density of liquid chemical at room temperature (g/cm <sup>3</sup> )

therefore:

$$D_w = 1.518 (10^{-4}) (M/d)^{-0.6} \quad (\text{A-11})$$

**A.2.2.1 Sulfur Mustard.** The molecular weight of HD is 159.02 and the liquid density is 1.27 g/cm<sup>3</sup>. At room temperature, the water diffusivity coefficient for sulfur mustard is:

$$D_w = 1.518 (10^{-4}) (159.02/1.27)^{-0.6} \quad (\text{A-12})$$

**A.2.2.2 Lewisite.** The molecular weight of Lewisite is 207.32 and the liquid density is 1.88 g/mL. At room temperature, the water diffusivity coefficient for Lewisite is:

$$D_w = 1.518 (10^{-4}) (207.32/1.88)^{-0.6} \quad (\text{A-13})$$

**A.2.2.3 Agent GA.** The molecular weight of GA is 162.1 and the liquid density is 1.09 g/ml. At room temperature, the water diffusivity coefficient for agent GA is:

$$D_w = 1.518 (10^{-4}) (162.1/1.09)^{-0.6} \quad (\text{A-14})$$

**A.2.2.4 Agent GB.** The molecular weight of GB is 140.1 and the liquid density is 1.09 g/ml. At room temperature, the water diffusivity coefficient for agent GB is:

$$D_w = 1.518 (10^{-4}) (140.1/1.09)^{-0.6} \quad (\text{A-15})$$

**A.2.2.5 Agent GD.** The molecular weight of GD is 182.2 and the liquid density is 1.02 g/ml. At room temperature, the water diffusivity coefficient for agent GD is:

$$D_w = 1.518 (10^{-4}) (182.2/1.02)^{-0.6} \quad (\text{A-16})$$

**A.2.2.6 Agent VX.** The molecular weight of VX is 267.37 and the liquid density is 1.0083 g/ml. At room temperature, the water diffusivity coefficient for agent VX is:

$$D_w = 1.518 (10^{-4}) (267.37/1.0083)^{-0.6} \quad (\text{A-17})$$

**A.2.3 Apparent Diffusivity.** The equation for deriving the apparent diffusivity ( $D_A$ ) of a chemical is as follows:

$$D_A = \frac{[(\Theta_a^{10/3} D_i H' + \Theta_w^{10/3} D_w)/n^2]}{\rho_b K_d + \Theta_w + \Theta_a H'} \quad (\text{A-18})$$

where (default values are given in parentheses):

$D_A$	=	Apparent diffusivity (cm <sup>2</sup> /s)
$\Theta_a$	=	Air-filled soil porosity (0.28 $L_{\text{air}}/L_{\text{soil}}$ , or $n - \Theta_w$ )
$D_i$	=	Diffusivity in air (cm <sup>2</sup> /sec), chemical specific (see below)
$H'$	=	Dimensionless Henry's Law Constant, chemical specific (41 x H)
$\Theta_w$	=	Water-filled soil porosity (0.15 $L_{\text{water}}/L_{\text{soil}}$ )
$D_w$	=	Diffusivity in water (cm <sup>2</sup> /sec), chemical specific (see below)
$n$	=	Total soil porosity (0.43 $L_{\text{air}}/L_{\text{soil}}$ , or $1 - (\rho_b/\rho_s)$ )
$\rho_b$	=	Dry soil bulk density (1.5 g/cm <sup>3</sup> )

$K_d$	=	Soil-water partition coefficient ( $\text{cm}^3/\text{g}$ ) = $K_{oc} \times f_{oc}$ )
$K_{oc}$	=	Soil-organic carbon partition coefficient (chemical specific)
$f_{oc}$	=	Percent organic carbon in soil (EPA Region IX default, 0.006)
$\rho_s$	=	Soil particle density ( $2.65 \text{ g/cm}^3$ )

**A.2.3.1 Sulfur Mustard.** The chemical-specific parameters for sulfur mustard are:  $D_i = 0.099$ ,  $H' = 8.61 \times 10^{-4}$ ,  $D_w = 8.4 \times 10^{-6}$ , and  $K_d = 0.798$ .

$$D_A = \frac{[(0.28)^{10/3} \times 0.099 \times 8.61 \times 10^{-4}] + [(0.15)^{10/3} \times 8.4 \times 10^{-6}]/(0.43)^2}{(1.5 \times 0.798) + 0.15 + (0.28 \times 8.61 \times 10^{-6})} \quad (\text{A-19})$$

$$D_A = 5 \times 10^{-6}$$

**A.2.3.2 Lewisite.** The chemical-specific parameters for Lewisite:  $D_i = 0.099$ ,  $H' = 1.31 \times 10^{-2}$ , and  $D_w = 9.0 \times 10^{-6}$ . A  $K_d$  cannot be estimated from a  $K_{ow}$  because the latter is not available due to rapid hydrolysis of the agent; therefore, the apparent diffusivity of Lewisite cannot be calculated.

**A.2.3.3 Agent GA.** The chemical-specific parameters for agent GA are:  $D_i = 0.092$ ,  $H' = 6.15 \times 10^{-6}$ ,  $D_w = 7.5 \times 10^{-6}$ , and  $K_d = 0.231$ .

$$D_A = \frac{[(0.28)^{10/3} \times 0.092 \times 6.15 \times 10^{-6}] + [(0.15)^{10/3} \times 7.5 \times 10^{-6}]/(0.43)^2}{(1.5 \times 0.231) + 0.15 + (0.28 \times 6.15 \times 10^{-6})} \quad (\text{A-20})$$

$$D_A = 2.35 \times 10^{-7}$$

**A.2.3.4 Agent GB.** The chemical-specific parameters for agent GB are:  $D_i = 0.10$ ,  $H' = 2.2 \times 10^{-5}$ ,  $D_w = 8.2 \times 10^{-6}$ , and  $K_d = 0.208$ .

$$D_A = \frac{[(0.28)^{10/3} \times 0.10 \times 2.2 \times 10^{-5}] + [(0.15)^{10/3} \times 8.2 \times 10^{-6}]/(0.43)^2}{(1.5 \times 0.208) + 0.15 + (0.28 \times 2.2 \times 10^{-5})} \quad (\text{A-21})$$

$$D_A = 5.4 \times 10^{-7}$$

**A.2.3.5 Agent GD.** The chemical-specific parameters for agent GD are:  $D_i = 0.082$ ,  $H' = 1.87 \times 10^{-4}$ ,  $D_w = 6.8 \times 10^{-6}$ , and  $K_d = 1.404$ .

$$D_A = \frac{[(0.28)^{10/3} \times 0.082 \times 1.87 \times 10^{-4}] + [(0.15)^{10/3} \times 6.8 \times 10^{-6}]/(0.43)^2}{(1.5 \times 1.404) + 0.15 + (0.28 \times 1.87 \times 10^{-4})} \quad (\text{A-22})$$

$$D_A = 5.57 \times 10^{-7}$$

**A.2.3.6 Agent VX.** The chemical-specific parameters for agent VX are:  $D_i = 0.062$ ,  $H' = 1.435 \times 10^{-7}$ ,  $D_w = 5.3 \times 10^{-6}$ , and  $K_d = 1.962$ .

$$D_A = \frac{[(0.28)^{10/3} \times 0.062 \times 1.43 \times 10^{-7}] + [(0.15)^{10/3} \times 5.3 \times 10^{-6}]/(0.43)^2}{(1.5 \times 1.962) + 0.15 + (0.28 \times 1.43 \times 10^{-7})} \quad (\text{A-23})$$

$$D_A = 1.68 \times 10^{-8}$$

### A.3 VOLATILIZATION FACTOR FOR SOIL ( $VF_s$ )

The equation for deriving the volatilization factor for soil ( $VF_s$ ) of a chemical is as follows:

$$VF_s = \left(\frac{Q}{C}\right) \times \frac{(3.14 \times D_A \times T)^{1/2}}{2 \times \rho_b \times D_A} \times 10^{-4} \text{ m}^2/\text{cm}^2 \quad (\text{A-24})$$

where (default values are given in parentheses):

$VF_s$	=	Volatilization Factor ( $\text{m}^3/\text{kg}$ )
$D_A$	=	Apparent diffusivity ( $\text{cm}^2/\text{s}$ )
$Q/C$	=	Inverse of the mean concentration at the center of a 0.5 acre square source ( $68.81 \text{ g/m}^2 \cdot \text{s}$ per $\text{kg/m}^3$ ).
$T$	=	Exposure interval ( $9.5 \times 10^8 \text{ sec}$ )
$\rho_b$	=	Dry soil bulk density ( $1.5 \text{ g/cm}^3$ )

**A.3.1 Sulfur Mustard.** The apparent diffusivity of HD is  $5 \times 10^{-6} \text{ cm}^2/\text{s}$ .

$$VF_s = 68.81 \times \frac{(3.14 \times 5 \times 10^{-6} \times 9.5 \times 10^8)^{1/2}}{2 \times 1.5 \times 5 \times 10^{-6}} \times 10^{-4} \quad (\text{A-25})$$

$$VF_s = 5.6 \times 10^4$$

**A.3.2 Agent GB.** The apparent diffusivity ( $D_A$ ) of agent GB is  $5.4 \times 10^{-7} \text{ cm}^2/\text{s}$ .

$$VF_S = 68.81 \times \frac{(3.14 \times 5.4 \times 10^{-7} \times 9.5 \times 10^8)^{1/2}}{2 \times 1.5 \times 5.4 \times 10^{-7}} \times 10^{-4} \quad (\text{A-26})$$

$$VF_S = 1.7 \times 10^5$$

**A.3.3 Agent GA.** The apparent diffusivity ( $D_A$ ) of agent GA is  $2.35 \times 10^{-7} \text{ cm}^2/\text{s}$ .

$$VF_S = 68.81 \times \frac{(3.14 \times 2.35 \times 10^{-7} \times 9.5 \times 10^8)^{1/2}}{2 \times 1.5 \times 2.35 \times 10^{-7}} \times 10^{-4} \quad (\text{A-27})$$

$$VF_S = 2.6 \times 10^5$$

**A.3.4 Agent GD.** The apparent diffusivity ( $D_A$ ) of agent GD is  $5.57 \times 10^{-7} \text{ cm}^2/\text{s}$ .

$$VF_S = 68.81 \times \frac{(3.14 \times 5.57 \times 10^{-7} \times 9.5 \times 10^8)^{1/2}}{2 \times 1.5 \times 5.57 \times 10^{-7}} \times 10^{-4} \quad (\text{A-28})$$

$$VF_S = 1.7 \times 10^5$$

**A.3.5 Agent VX.** The apparent diffusivity ( $D_A$ ) of agent VX is  $1.68 \times 10^{-8} \text{ cm}^2/\text{s}$ .

$$VF_S = 68.81 \times \frac{(3.14 \times 1.68 \times 10^{-8} \times 9.5 \times 10^8)^{1/2}}{2 \times 1.5 \times 1.68 \times 10^{-8}} \times 10^{-4} \quad (\text{A-29})$$

$$VF_S = 9.7 \times 10^5$$

#### A.4 SOIL SATURATION LIMIT ( $C_{\text{sat}}$ )

The soil saturation limit ( $C_{\text{sat}}$ ) is the contaminant concentration at which soil pore air and pore water are saturated with the chemical and the adsorptive limits of the soil particles have been reached (USEPA, 1996c). Above this concentration, the contaminant exists in the soil in the free phase, and Equation 2-1 cannot be used to estimate the Volatilization Factor. VF-based screening levels are not accurate for concentrations above the  $C_{\text{sat}}$ . The  $C_{\text{sat}}$  for each chemical can be estimated as follows (USEPA, 1996c):

$$C_{\text{sat}} = \frac{S}{\rho_b} (K_d \rho_b + \Theta_w + H'\Theta_a) \quad (\text{A-30})$$

where:

$C_{\text{sat}}$	=	Soil Saturation concentration (mg/kg)
$S$	=	Solubility in water (mg/L), chemical specific
$\rho_b$	=	Dry soil bulk density (1.5 kg/L)
$K_d$	=	Soil-water partition coefficient $[(\text{cm}^3/\text{g}) = K_{\text{oc}} \times f_{\text{oc}}]$
$K_{\text{oc}}$	=	Soil organic carbon-water partition coefficient (chemical-specific), used to calculate $K_d$
$f_{\text{oc}}$	=	Percent organic carbon in soil (EPA Region IX default, 0.006)
$\Theta_w$	=	Water-filled soil porosity ( $0.15 L_{\text{water}}/L_{\text{soil}}$ )
$H'$	=	Dimensionless Henry's Law Constant, chemical-specific ( $41 \times$ Henry's Law Constant)
$\Theta_a$	=	Air-filled soil porosity ( $0.28 L_{\text{air}}/L_{\text{soil}}$ , or $n - \Theta_w$ )
$n$	=	Total soil porosity [ $0.43 L_{\text{air}}/L_{\text{soil}}$ , or $1 - (\rho_b/\rho_s)$ ]
$\rho_s$	=	Soil particle density ( $2.65 \text{ g/cm}^3$ ), used to calculate $n$

The EPA default values are given in parentheses. Soil saturation limits for the chemical agents are listed in Table 2-3. Agent GB is miscible with water. A soil saturation limit cannot be derived for Lewisite because of the rapid hydrolysis of the compound.

## A.5 PARTICULATE EMISSION FACTOR (PEF)

Inhalation of fugitive dusts is an exposure pathway that is considered in deriving Preliminary Remediation Goals and Soil Screening Levels (SSLs). Derivation of a fugitive dust SSL requires calculation of a PEF that relates the concentration of the chemical in soil to its concentration in dust particles in air. The PEF represents an annual average emission rate based on wind erosion. The PEF is calculated as follows:

$$PEF = \left(\frac{Q}{C}\right) \times \frac{3,600 \text{ sec/hr}}{0.036 \times (1 - V) \times (U_m/U_t) \times F(x)} \quad (\text{A-31})$$

where:

PEF	=	Particulate emission factor ( $1.32 \times 10^9 \text{ m}^3/\text{kg}$ )
$Q/C$	=	Inverse of the mean concentration at the center of a 0.5 acre square source ( $90.80 \text{ g/m}^2 \cdot \text{s}$ per $\text{kg/m}^3$ )
$V$	=	Fraction of vegetative cover (50%)
$U_m$	=	Mean annual wind speed (4.69 m/s)
$U_t$	=	Equivalent threshold value of windspeed at 7 m (11.32 m/s)
$F(x)$	=	Function dependent on $U_m/U_t$ ; see Cowherd et al., 1985 (0.194)

## APPENDIX B

### CARCINOGENIC POTENCY FOR SULFUR MUSTARD

This Appendix contains a copy of a letter received from Dr. David Gaylor, National Center for Toxicological Research, Food and Drug Administration, Jefferson, Arkansas. Dr. Gaylor had previously made comments and shared his expertise regarding various approaches to evaluating the carcinogenic potency of chemicals. As a member of the National Research Council Committee on Toxicology (COT), Subcommittee on Chronic Reference Doses for Selected Chemical Warfare Agents, reviewing chronic toxicological data for the chemical warfare agents, he was familiar with the available toxicity data for sulfur mustard. The Army requested that Dr. Gaylor provide documentation of his own evaluation of the carcinogenic potency of sulfur mustard.





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March 11, 1998

Ms. Veronique Hauschild  
Hazardous and Medical Waste Program  
U.S. Army Center for Health Promotion  
and Preventive Medicine  
Bldg. E-1675  
Aberdeen Proving Ground, MD 21010-5422

Dear Ms. Hauschild:

Dr. Annetta Watson, Oak Ridge National Laboratory, asked me to share with you my analysis of the potential cancer risk from long-term, low-dose oral exposure to sulfur mustard (enclosed). As you know, this is one of the agents being evaluated by a National Research Council subcommittee. That subcommittee is still evaluating sulfur mustard and other agents. Hence, the enclosed comments are strictly my own at this time and do not necessarily represent those of the subcommittee. This material has been submitted to the subcommittee, but it could undergo substantial revision review conducted by the National Research Council.

I would be available to discuss this material further with you. I can be reached by telephone: [870] 543-7001; fax: [870] 543-7576; and e-mail: [dgaylor@nctr.fda.gov](mailto:dgaylor@nctr.fda.gov).

Sincerely,

David W. Gaylor, Ph.D.  
Assoc. Dir. for Risk Assessment  
Policy and Research  
NCTR/FDA

Enclosure

cc:  
Dr. Annetta Watson, Oak Ridge National Laboratory  
Dr. Kulbir Bakshi, National Research Council

Revised for Army

# **Carcinogenic Potency for Sulfur Mustard**

**D.W. Gaylor, Ph.D.**

**March 11, 1998**

There are a number of human studies that provide estimates of the relative risk for cancer associated with exposure to sulfur mustard. The duration of exposure is reported for some of these studies, but there was no indication of the dose levels. Hence, it is not possible to estimate the carcinogenic potency (risk per mg/kg-d) from the reported human data.

There has not been a chronic study in which animals were administered sulfur mustard orally. However, there are several indirect methods for estimating the carcinogenic potency of sulfur mustard. These are summarized in the following discussion.

Watson et al. (1989) argue that the carcinogenic potency of sulfur mustard is 1.3 times that of benzo(a)pyrene. The carcinogenic potency of benzo(a)pyrene listed in the USEPA Integrated Risk Information System is less than 7.3 per mg/kg-d. Hence, the estimated carcinogenic potency for sulfur mustard is less than  $1.3 \times 7.3 = 9.5$  per mg/kg-d by this approach.

In a recent chronic feeding study of benzo(a)pyrene conducted in B6C3F1 female mice (Culp et al., 1998), the incidence of forestomach tumors were 1/48, 3/47, 36/46, and 46/47 at 0, 5, 26, and 100 ppm, respectively. The carcinogenic potency of benzo(a)pyrene was estimated to be less than 1.2 per mg/kg-d, assuming equal potency between animals and humans for dose adjusted by body weight to the  $3/4$  power. Note that this is  $1/6$  of the current USEPA potency value for benzo(a)pyrene. If sulfur mustard is 1.3 times more potent than benzo(a)pyrene (Watson et al., 1989), the carcinogenic potency for sulfur mustard is estimated to be less than  $1.3 \times 1.2 = 1.6$  per mg/kg-d based on the carcinogenicity of benzo(a)pyrene observed by Culp et al. (in press).

Sasser et al. (1989a) observed forestomach hyperplasia in male and female Sprague-Dawley rats gavaged with sulfur mustard in sesame oil, 5 days per week for 13 weeks. The incidence of hyperplasia was 0/24, 0/24, 0/24, 0/24, 1/24, and 10/24 at 0, 0.003, 0.01, 0.03, 0.1, and 0.3 mg/kg-d, respectively. Making the conservative assumption that hyperplasia at 13 weeks may serve as a biomarker for potential tumorigenicity, the multistage model was fit to these data providing an estimate of 10% incidence at 0.16 mg/kg-d. The lower 95% confidence limit on this dose was 0.10 mg/kg-d. Adjusting this dose for gavaging on 5 days per week and body weight to the  $3/4$  power results in a lower confidence limit of 0.02 mg/kg-d. In accordance with the proposed carcinogen risk assessment guidelines (USEPA, 1996), linear extrapolation to zero gives a potential carcinogenic potency of less than  $0.1/0.02 = 5.0$  per mg/kg-d.

Sasser et al. (1989b) observed benign forestomach lesions in male and female Sprague-Dawley rats gavaged in a two-generation reproductive study with sulfur mustard. The incidence of lesions was 0/94, 0/94, 8/94, and 10/94 at 0, 0.3, 0.1, and 0.4 mg/kg-d. Making the conservative assumption that these lesions may serve as a biomarker for potential tumorigenicity, the multistage model was fit to these data providing a 10% incidence at 0.28 mg/kg-d, with a lower 95% confidence limit of 0.19 mg/kg-d. Adjusting this dose for gavage on 5 days per week and body weight to the  $3/4$  power results in a lower confidence limit of 0.038

mg/kg-d. Following the proposed carcinogen risk assessment guidelines (USEPA, 1996), linear extrapolation to zero gives a potential carcinogenic potency of less than  $0.1/0.038 = 2.6$  per mg/kg-d of sulfur mustard.

Gaylor and Gold (1995) observed for 139 animal carcinogens tested in the National Toxicology Program that carcinogenic potency can be estimated by 0.74 divided by the maximum tolerated dose, expressed in terms of mg/kg-d. Sasser et al. (1989a) reported significant body weight depression in rats administered 0.3 mg/kg-d sulfur mustard for 90 days. No toxic effects were noted at 0.1 mg/kg-d. Hence, a dose of 0.2 mg/kg-d might serve as the maximum dose in a 2-year study. With a maximum tolerated dose of 0.2 mg/kg-d for 5 days per week, the average daily dose at the maximum tolerated dose of  $0.2 \times (5/7) = 0.14$  mg/kg-d. From Gaylor and Gold (1995), an estimate of the carcinogenic potency is less than  $0.74/0.14 = 5.3$  per mg/kg-d of sulfur mustard.

In the absence of a chronic bioassay for sulfur mustard, these diverse methods for estimating an upper limit on the carcinogenic potency gave remarkably similar results of 1.6 to 9.5 per mg/kg-d for lifetime exposure (Table B). I would expect a 2-year rodent bioassay to yield results in or near this range. Cancer risk is estimated to be less than the carcinogenicity potency times the average lifetime daily dose. For example, if it were desired to restrict the potential carcinogenic risk from ingestion of sulfur mustard to less than  $10^{-5}$  for those individuals exposed for a lifetime, daily oral doses should probably be limited to  $10^{-5}/1.6 = 6 \times 10^{-6}$  mg/kg-d to  $10^{-5}/9.5 = 1 \times 10^{-6}$  mg/kg-d. This is about the same range of doses derived for the reference dose for noncancer effects.

<b>Table B-1. Estimates of the upper limit for carcinogenic potency (risk per mg/kg-d) of sulfur mustard</b>	
<b>Method of Estimation</b>	<b>Estimate</b>
Potency relative to benzo(a)pyrene potency from the USEPA IRIS (Watson et al., 1989)	9.5
Potency relative to benzo(a)pyrene potency from Culp et al. (1998)	1.6
Linear extrapolation from the benchmark dose of forestomach hyperplasia (Sasser et al., 1989a)	5.0
Linear extrapolation from the benchmark dose of forestomach lesions (Sasser et al., 1989b)	2.6
Relative to the maximum tolerated dose (Gaylor and Gold, 1995)	5.3

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## APPENDIX C

### SCREENING VALUES FOR TRESPASSERS

#### C.1 OBJECTIVE

The objective of this section is to provide an example of how the Preliminary Remediation Goal (PRG) and Risk Based Concentration (RBC) models can be used to evaluate potential chronic health risks to trespassers from exposures to soil containing residual chemical warfare agents sulfur mustard (HD) and Lewisite, and the nerve agents Tabun (GA), Sarin (GB), Soman (GD), and VX.

The example provided is a theoretically-based scenario which uses assumptions that are intended to be reasonably conservative. However, parameter values used in the trespasser scenario are highly variable in real-world situations. Therefore, site-specific risk assessment in these scenarios is advised. The values chosen for these examples, though intended to be conservative, may not be sufficiently conservative for all situations, while in other circumstances, the application of the risk assessment model itself may not be appropriate. For example, if conditions exist such that trespasser exposures may be as high as 50 days each year, then the values used in these examples (12 days each year) would not be conservative enough. On the other hand, other real-world exposure scenarios may not present a chronic/repeated exposure problem (i.e., if trespassers do not regularly and repeatedly come in contact with soil containing agent), then application of a U.S. Environmental Protection Agency (USEPA) chronic risk assessment model (e.g., PRG) is not appropriate or necessary.

#### C.2 BACKGROUND

For military sites that have restricted access, there exists the possibility that the site might be visited by unauthorized individuals (trespassers). In order to assess the potential health risks to such individuals, theoretical scenarios were developed based on approaches used in previous Department of Defense (DOD) risk assessments and on recommendations made by USEPA. Two trespasser scenarios are evaluated in this report; one considers adolescents (from age 7 up to and including 16; covering a 10-year exposure period) as the most likely trespassers (USEPA Region IV approach), and the second considers adult hunters or fishermen as being potential trespassers. In the latter case, the assumption is also made that the same individuals may be exposed as both adolescents (starting at age 7) and adults (starting at age 17 and continuing until age 30). Age 30 is selected as the endpoint because USEPA considers 30 years as a reasonable maximum residency period at any one location. Therefore, the total exposure duration for the adolescent/adult category is 23 years (i.e., starting at age 7 up to age 30).

#### C.3 METHOD

The general USEPA Region IX risk assessment methodology for deriving PRGs (see Sections 3.2.5 and 3.2.6) for industrial soil (USEPA, 1996b) and the USEPA Region III risk assessment methodology for deriving RBCs (see Sections 3.1.3 and 3.1.4) for industrial soil (USEPA, 1996a) will be used to calculate Health-Based Environmental Screening Levels for trespassers (HBESL<sub>tres</sub>) for the chemical agents.

The Region IX method includes potential exposure by three routes: ingestion of soil, dermal contact, and inhalation of volatiles or particulates released from the soil. For noncancer endpoints, the algorithm for calculating a screening value for a trespasser is as follows:

$$HBESL_{tres} = \frac{THQ \times BW_t \times AT_n}{EF_t \times ED_t \times \left( \left( \frac{1}{RfD_o} \times \frac{IRS_t}{10^6 \text{ mg/kg}} \times FC \right) + \left( \frac{1}{RfD_o} \times \frac{SA_t \times AF \times ABS}{10^6 \text{ mg/kg}} \right) + \left( \frac{1}{RfD_i} \times \frac{IRA_t \times ET_t}{VF_s} \right) \right)}$$

(C-1)

where:

HBESL <sub>tres</sub>	=	Health-based Environmental Screening Level for trespasser (mg chemical/kg soil)
THQ	=	Toxicity Hazard Quotient (=1)
BW <sub>t</sub>	=	Body weight (kg)
AT <sub>n</sub>	=	Averaging time, noncarcinogens (ED x 365 days/yr)
EF <sub>t</sub>	=	Exposure frequency (days/yr)
ED <sub>t</sub>	=	Exposure duration (yr)
RfD <sub>o</sub>	=	Oral Reference Dose (mg chemical/kg body weight/day)
RfD <sub>d</sub>	=	Dermal Reference Dose (mg/kg/day) <b>for Lewisite only</b> (see Section 9.2)
IRS <sub>t</sub>	=	Soil ingestion rate (mg/day)
FI	=	Fraction ingested from contaminated source
SA <sub>t</sub>	=	Skin surface area exposed (cm <sup>2</sup> )
AF	=	Soil-to-skin adherence factor (mg/cm <sup>2</sup> )
ABS	=	Skin absorption factor (%)
RfD <sub>i</sub>	=	Inhalation Reference Dose (mg chemical/kg/day)
IRA <sub>t</sub>	=	Inhalation rate (m <sup>3</sup> /day)
ET <sub>t</sub>	=	Fraction of day spent at site
VF <sub>s</sub>	=	Chemical-specific volatilization factor for soil (m <sup>3</sup> /kg)

According to USEPA guidelines, for contaminants having a Henry's Law Constant of less than 10<sup>-5</sup> atm-m<sup>3</sup>/mol, the Volatilization Constant in Equation C-1 is replaced with a default Particulate Emission Factor (PEF) of 1.32 x 10<sup>9</sup> m<sup>3</sup>/kg (USEPA, 1996b). This applies to all the nerve agents. A PEF is also used for Lewisite because a chemical-specific Volatilization Factor (VF) cannot be calculated because a K<sub>ow</sub> is not available. The inhalation of volatiles pathway was included for all the agents, even though the only agent of those evaluated in this report that may be expected to volatilize from subsurface soils is HD. Volatilization was considered to be a potentially important exposure pathway in the case of trespassers because of the possibility that the shortened exposure frequencies would allow for relatively high residual agent concentrations in soil.

For contaminants having a carcinogenic effect, the algorithm used to calculate a screening value for a trespasser is as follows:

$$HBESL_{tres} = \frac{THQ \times BW_t \times AT_c}{ED_t \times EF_t \times \left( \left( \frac{IRS_t \times CSF_o \times FC}{10^6 \text{ mg/kg}} \right) + \left( \frac{SA_t \times AF \times ABS \times CSF_o}{10^6 \text{ mg/kg}} \right) + \left( \frac{IRA_t \times ET_t \times CSF_i}{VF_s} \right) \right)} \quad (C-2)$$

where:

$HBESL_{tres}$	=	Health-Based Environmental Screening Level for trespasser (mg chemical/kg soil)
TR	=	Target cancer risk
$BW_t$	=	Body weight (kg)
$AT_c$	=	Averaging time for carcinogenic effects (70 yr)
$ED_t$	=	Exposure duration (yr)
$EF_t$	=	Exposure frequency (days/yr)
$IRS_t$	=	Soil ingestion (mg/day)
$CSF_o$	=	Oral slope factor [(mg/kg/day) <sup>-1</sup> ]
FI	=	Fraction ingested from contaminated source
$SA_t$	=	Skin surface area exposed (cm <sup>2</sup> )
AF	=	Adherence factor (mg/cm <sup>2</sup> )
ABS	=	Skin absorption factor (percent)
$IRA_t$	=	Inhalation rate (m <sup>3</sup> /day)
$ET_t$	=	Fraction of day spent at site
$CSF_i$	=	Inhalation slope factor [(mg/kg/day) <sup>-1</sup> ]
$VF_s$	=	Volatilization factor for soil, chemical-specific (m <sup>3</sup> /kg)
PEF	=	Particulate emission factor for soil (1.32 x 10 <sup>9</sup> m <sup>3</sup> /kg)

Rationales for the exposure parameter values unique to the  $HBESL_{tres}$  calculations are presented below. All the parameters used in Equations C-1 and C-2 are presented in Table C-1.

**Dermal Reference Dose (RfDd).** Derived for Lewistite using acute toxicity data (See Section 9.2).

**Target cancer risk (TR).** A discussion of the use of target cancer risk levels is given in Section 1.3.2 of this document. The target cancer risk level of 10<sup>-5</sup> that is used for residential exposure scenarios is also considered appropriate for the trespasser scenarios.

**Body weight (BW<sub>t</sub>).** USEPA Region IV considers the typical trespasser to be an adolescent 7-16 years old with a body weight of 45 kg (USEPA, 1995b). For the trespasser scenario for both adolescents and adults, an age span of 7-30 years and an average body weight of 60 kg is used in this report (estimated from age-specific body weight data provided in USEPA, 1989a).

**Exposure Duration (ED<sub>t</sub>).** The only USEPA guidelines for selecting exposure duration values for trespassers is the default recommended by USEPA Region IV that the most likely adolescent trespassers would be 7-16 years old, resulting in a 10-year exposure duration. Other exposure durations may be more appropriate for specific sites. If a site includes habitat populated by game animals or includes lakes or streams populated with fish, it may be attractive to hunters or fishermen. The possibility would then exist



that the trespasser will be an adult and that the exposure duration will extend over a longer period of time, possibly as long as the individuals live in the area. Using the standard residential exposure duration of 30 years, an adolescent/adult trespasser exposure duration of 23 years is recommended (i.e., 10 years for adolescents age 7-16 and 13 years for adults age 17-30). The total 30-year period corresponds to the maximum reasonable residential duration from birth to age 30 at a single site.

**Exposure Frequency (EF<sub>t</sub>).** USEPA Region IV notes that selection of trespasser exposure frequency should consider site-specific factors such as distance from the site to residences and the attractiveness of the site to the trespasser. For the purposes of this report, an exposure frequency of 12 days per year was chosen for the trespasser scenario. Other exposure frequencies may be more appropriate for specific sites, depending on climate, site accessibility, and the use of the site by hunters or fishermen.

**Exposure Time (ET<sub>t</sub>).** There are no USEPA default values for the length of time that trespassers will remain at a given site. For the purposes of this report, an exposure time of 1 hour is used. Other exposure times may be more appropriate for specific sites.

**Soil Ingestion rate (IRS<sub>t</sub>).** The standard default for daily soil ingestion by individuals older than 6 years is 100 mg/day, and this value is used here for soil ingestion by trespassers.

**Fraction ingested from source (FI).** This parameter reflects the percentage of daily ingested soil that contains the chemical agent of concern. Since the IRS<sub>t</sub> reflects the daily rate of soil ingestion, it includes ingestion of soils and dusts from sources outside of the restricted area. It is assumed here that 50% of the daily ingested soil will come from the site.

**Skin surface area exposed (SA<sub>t</sub>).** For the adolescent trespasser scenario used in this report, an exposed skin surface area of 4300 cm<sup>2</sup>, the median value between children and adults, is used. For the adolescent/adult trespasser, an exposed skin surface area of 5000 cm<sup>2</sup>, the median value between adolescents and adults, is used.

Table C-1. Values used for calculating trespasser HBESLs			
Parameter	Value	Source	Comment/Reference
THQ	1	USEPA	Standard USEPA value (RAGs Part A, 1989; Part B, 1991a)
RfD <sub>o</sub>	Chemical-specific	Army	Interim standard (Army Office of the Surgeon General, August 1, 1996; see Table 1-2).
RfD <sub>i</sub>	Chemical-specific	Army	Derived from Air Exposure Limits (see Table 1-2) adopted by DHHS (1988) and by the Army (DA, 1990; 1991) using an inhalation rate of 20 m <sup>3</sup> /day and a body weight of 70 kg.
RfD <sub>a</sub>	Chemical-specific	Army	Used for Lewisite only. Derived from acute toxicity data (see Sections 1.2 and 9.2).
CSF <sub>o</sub>	Chemical-specific	Army	See Table 1-2.
CSF <sub>i</sub>	Chemical-specific	Army	See Table 1-2.
TR	10 <sup>-5</sup>	Army	The recommended range of values is 10 <sup>-4</sup> to 10 <sup>-6</sup> (RAGs part A). A TR of 10 <sup>-5</sup> is used in this report for residential exposures (see Section 1.3.2)
BW	45 kg 60 kg	Army	Adolescents (see text) Adolescents/adults (see text)
AT <sub>c</sub>	25,550 days	USEPA	The AT for carcinogenic risks is assumed to be over a lifetime (70 yr) because it is the additional risk averaged over the lifetime of the individual(s) exposed (RAGs, Part A).
AT <sub>n</sub>	ED	USEPA	For noncarcinogenic risks the AT equals the duration of exposure (ED) (RAGs Part A and Part B)
EF <sub>t</sub>	12 days/yr	Army	See text
ED <sub>t</sub>	10 yr 23 yr	Army	Adolescents (see text) Adolescents/adults (see text)
ET <sub>t</sub>	1 hr	Army	See text
IRS <sub>t</sub>	100 mg/day	Army	Standard USEPA default for soil ingestion by adults
FI	0.5	USEPA	Fraction of daily soil ingested from site
SA <sub>t</sub>	4300 cm <sup>2</sup> 5000 cm <sup>2</sup>	Army	Adolescents (see text) Adolescents/adults (see text)
ABS	Chemical-specific	Army	For 12-hour period (see Table 2-4)
AF	0.08 mg/cm <sup>2</sup>	USEPA	This value is used for adults by USEPA Region IX
IRA <sub>t</sub>	20 m <sup>3</sup> /day	Army	Standard USEPA default for adults
VF	Chemical-specific	Army	Calculated using USEPA recommended methods (see Table 2-3)
PEF	1.32 x 10 <sup>9</sup> m <sup>3</sup> /kg	USEPA	Standard USEPA default (USEPA, 1996c)

## C.4 RESULTS

The trespasser HBESL values calculated with Equations C-1 and C-2, using the toxicity values listed in Table 1-2 and the exposure parameters listed in Table C-1, are summarized in Table C-2. To use these values as an action/no action tool, the application criteria bulleted below must be met. In addition, the user should be familiar with the key uncertainties (identified in Table C-3) in the assessment model and type of effect. In this type of scenario, types of 'action' that may be determined to be necessary include additional management/engineering controls, treatment to further minimize potential for repeated/long-term exposure, or site-specific risk assessment to ascertain specific exposure conditions.

*Target risk levels are acceptable*

This can only be assessed through negotiation with applicable regulators and other stakeholders (see Section 1.3.2).

*Assumptions made in these scenarios are at least equally conservative if not more conservative than site-specific assumptions.*

For example, if a site-specific scenario includes an exposure frequency of more than 12 days/yr, then the HBESL assumption may be considered under-conservative.

*Exposure frequency and duration represent a chronic exposure.*

Since exposure durations and frequencies cited in the example may not be realistically considered a significant chronic or even subchronic exposure, the application of a chronic risk model may be inappropriate. In such cases acute toxicity should be evaluated separately (see Section C.5).

*A single chemical agent is of concern.*

<b>Table C-2. Calculated HBESL<sub>tres</sub> values for chemical warfare agents</b>					
<b>Agent</b> (mg/kg soil)	<b>Scenario</b>	<b>PRG</b> (noncancer)	<b>PRG<sup>a</sup></b> (cancer)	<b>RBC</b> (noncancer)	<b>RBC<sup>a</sup> (cancer)</b>
HD	adolescent	119 <sup>b</sup>	19 <sup>b</sup>	192	249
	adolesc./adult	150 <sup>b</sup>	11 <sup>b</sup>	256	144
Lewisite	adolescent	66	-	27*	-
	adolesc./adult	76	-	36*	-
GA	adolescent	451 <sup>b</sup>	-	1095	-
	adolesc./adult	583 <sup>b</sup>	-	1460	-
GB	adolescent	225 <sup>b</sup>	-	548	-
	adolesc./adult	294 <sup>b</sup>	-	730	-
GD	adolescent	42 <sup>b</sup>	-	110	-
	adolesc./adult	54 <sup>b</sup>	-	146	-
VX	adolescent	13 <sup>b</sup>	-	16.4	-
	adolesc./adult	17 <sup>b</sup>	-	21.9	-

<sup>a</sup> Target cancer risk level of 10<sup>-5</sup>

<sup>b</sup> Inhalation of vapors included in calculation

\* Calculated values decreased by a factor of 100 to compensate for possibility of acute toxicity (see text)

Table C-3. Uncertainty Summary - Key Areas of Uncertainty and Type of Effect* on "Conservatism" of HBESL <sub>tres</sub>	
Type of Uncertainty	Type of effect
Inhalation slope factor (CSF <sub>i</sub> )	Possible over conservatism because of route-to-route extrapolation
Multiple exposure pathways (PRG)	Possible over conservatism, especially for vesicants HD and Lewisite
Exposure duration (ED <sub>i</sub> )	Unknown - possible over/under conservatism
Exposure frequency (EF <sub>i</sub> )	Unknown - possible over/under conservatism
Exposure time (ET <sub>i</sub> )	Unknown - possible under conservatism
Skin surface area exposed (SA)	Unknown - depends on climate and season of the year
Fraction ingested from contaminated source (FI)	Unknown - possible over/under conservatism
Acute toxicity	Possible under conservatism, but compensated for by using an adjustment factor of 10

\* Type of effect has been determined by professional judgement

## C.5 HBESL<sub>tres</sub> COMPARISONS WITH ACUTE TOXICITY DATA

Because the calculated HBESL<sub>tres</sub>s are extrapolations from chronic toxicity values to relatively short-term exposures, care must be used to ensure that the resulting criteria are not set at levels at which acute toxic effects might occur. The chronic risk assessment model may fail to accommodate the 'acute' risk from a single 'hotspot' of concentrated chemical agent. In situations where the calculated HBESL is at levels which approach potential acute toxicity concerns, it may be more prudent to consider the assessment of individual hotspots to ensure that the potential of acute risk is mitigated at these higher concentration levels. Only in situations where the agent is reasonably assumed to be homogeneously adsorbed or otherwise mixed in with the matrix (e.g. possibly waste soil or even more homogenous as in liquid matrices) is the use of the risk assessment model appropriate.

In this section the potential exposures at the trespasser HBESLs are compared to experimental human and animal data identifying no-effect and minimum effect levels (MELs) for acute exposures. The acute toxicity data are summarized in more detail in Section 1.3.8. It should be noted that the potential for acute toxicity is dependent on the values used for the exposure parameters.

**Agent HD.** The maximum HBESL<sub>tres</sub> is 256 mg HD/kg soil for adolescents/adults. At this HBESL, the dose resulting from the incidental ingestion of 50 mg of soil is approximately 0.0013 mg HD (0.0002 mg/kg body weight). In studies conducted on rats, a dose of 0.03 mg/kg/day (about 0.01 mg/animal) caused no toxic effects or produced only mild signs of toxicity after repeated exposures for 13 weeks (see Section 1.3.8).

Assuming an exposed skin area of 5000 cm<sup>2</sup> for adolescent/adult trespassers, and a soil-to-skin adherence of 0.08 mg per cm<sup>2</sup> of skin, the amount of soil that may be in contact with the skin is 400 mg and, at the maximum HBESL<sub>tres</sub> of 256 mg/kg, this quantity of soil would contain about 0.1 mg of HD (256 mg/kg x 1 kg/1,000,000 mg x 400 mg). The average amount of HD per square centimeter of exposed skin would be 0.02 µg (0.01 mg/5000 cm<sup>2</sup>). In human experimental studies application of 2.5 µg of HD to the skin resulted in erythema, in 87 of 209 individuals and blistering in 5 of 209 (see Section 1.3.8). These data indicate that

the minimum effect level may be less than 1  $\mu\text{g}$ ; in comparison, at the HBESL, the estimated average exposure is 0.02  $\mu\text{g}/\text{cm}^2$  (and it would be about one-tenth of this value for the cancer-based HBESL<sub>tres</sub> values). These HBESLs would be marginally protective of acute percutaneous exposures, but only if the agent is uniformly dispersed in the soil. The HBESL<sub>tres</sub> values should not be applied to situations where the HD is concentrated in “hotspots” or where globules of agent are encapsulated in a polymeric coating formed by the HD hydrolysis products (see Section 1.2.3).

The HBESL (256 mg/kg) could theoretically result in an HD air concentration of 0.005 mg/m<sup>3</sup>, assuming that the air concentration is a function of the soil concentration (256 mg/kg) divided by the VF (5.62 x 10<sup>4</sup> m<sup>3</sup>/kg). A CT of 12 mg-min/m<sup>3</sup> (0.2 mg/m<sup>3</sup> for 60 min) has been reported to be a no-effect level for eye irritation (see Section 1.3.8). The maximum allowable CT for skin effects is 5 mg-min/m<sup>3</sup> and that for eye effects is 2 mg-min/m<sup>3</sup> (DA, 1974); these values equate to 0.08 and 0.03 mg/m<sup>3</sup>, respectively, for 60-min exposures. Therefore, for the presumed conditions of exposure for the trespasser scenario (i.e., 1-hr exposure time), if the resulting air concentration is no greater than 0.0005 mg/m<sup>3</sup>, then the HBESLs appear to be sufficiently protective against the possibility of vapor effects to the skin or eyes.

**Agent VX.** The maximum HBESL<sub>tres</sub> is 22 mg VX/kg soil for adolescent/adults, and the dose resulting from the incidental ingestion of 50 mg of soil would be approximately 0.0001 mg VX. In tests on humans, an oral dose of about 0.1 mg (calculated from a reported dose of 0.0014 mg/kg/day and a default body weight of 70 kg) caused no signs of toxicity even after 7 days of exposure (see Section 1.3.8). This dose is about 100 times greater than that estimated from the maximum soil HBESL<sub>tres</sub>, under the assumed conditions of exposure.

VX is not very volatile; therefore, the percutaneous and oral exposures are expected to be much more significant than the inhalation exposure. Assuming an exposed skin area of 5000 cm<sup>2</sup> for adolescent/adult trespassers, and a soil-to-skin adherence of 0.08 mg per cm<sup>2</sup> of skin, the amount of soil that may be in contact with the skin is 400 mg and, at the HBESL<sub>tres</sub> of 22 mg/kg, this quantity of soil would contain about 0.009 mg of VX [22 mg/kg x (1 kg/1,000,000 mg) x 400 mg = 0.009 mg VX]. In comparison, DA (1974) reported that 0.32 mg of liquid VX applied to the forearm resulted in mild signs of toxicity in 1% of the tested individuals. Therefore, acutely toxic effects are not likely at the HBESL, under the stated conditions of exposure.

**Agent GB.** The maximum HBESL<sub>tres</sub> is 730 mg GB/kg soil for adolescent/adults, and the dose resulting from the incidental ingestion of 50 mg of soil would be approximately 0.037 mg GB. In tests on humans, an oral dose of about 1.54 mg (based on a reported dose of 0.022 mg/kg/day and a default body weight of 70 kg) caused mild signs of toxicity (see Section 1.3.8). A dose of 0.15 (based on a reported dose of 0.002 mg/kg/day and a default body weight of 70 kg) caused only excessive dreaming and talking in sleep (see Section 1.3.8). Therefore, the HBESL<sub>tres</sub> would appear to be protective for acute oral toxicity under the stated conditions of exposure.

Assuming a soil adherence of 0.08 mg per cm<sup>2</sup> of skin and a total exposed skin area of 5000 cm<sup>2</sup>, the total amount of soil on the skin would amount to 400 mg. At the maximum HBESL<sub>tres</sub> of 730 mg GB/kg soil for adolescent/adults, 0.3 mg of GB would be in contact with the skin [730 mg/kg x (1 kg/1,000,000 mg) x 400 mg = 0.3 mg GB]. In comparison, it has been reported that 20-50 mg of GB applied to the skin will not result in signs of toxicity (see Section 1.3.8); therefore, the soil HBESL<sub>tres</sub> levels should be protective of acute dermal exposures for the stated conditions of exposure.

A soil HBESL of 730 mg/kg soil could theoretically result in a GB air concentration of 0.004 mg/m<sup>3</sup>, assuming that the air concentration can be estimated from the soil concentration (730 mg/kg) divided by the VF ( $1.7 \times 10^5$  m<sup>3</sup>/kg). The estimated no-effect concentration for a 60-min exposure to GB is 0.02 mg/m<sup>3</sup> (see Section 1.3.8), therefore, it is unlikely that the soil trespasser HBESLs would result in an acutely toxic vapor concentrations, for the assumed conditions of exposure.

**Agent GA.** The maximum HBESL<sub>tres</sub> is 1460 mg/kg for adolescents/adults. At this HBESL, the dose resulting from ingestion of 50 mg of soil is about 0.07 mg GA. A minimum effect level in humans is estimated to be 0.37 mg (see Section 1.3.8); therefore, the soil HBESL<sub>tres</sub> levels are expected to be marginally protective for acute toxicity resulting from incidental ingestion of soil, for the stated conditions of exposure.

At the maximum HBESL<sub>tres</sub> of 1460 mg/kg soil for adolescent/adults, and assuming a soil adherence of 0.08 mg per cm<sup>2</sup> of skin and a total exposed skin area of 5000 cm<sup>2</sup>, the total amount of soil on the skin would amount to 400 mg and would contain 0.6 mg of GA [1460 mg/kg x (1 kg/1,000,000 mg) x 400 mg = 0.6 mg GA]. In comparison, it was estimated that the minimum effect level for dermal exposures is 32-48 mg, and experimental data suggest that it may be as high as 300 mg (see Section 1.3.8). This is substantially greater than the maximum dermal dose for trespassers; therefore, the soil HBESL<sub>tres</sub> levels would appear to be protective of acute dermal exposures for the stated conditions of exposure.

A soil HBESL of 1460 mg/kg soil could theoretically result in a GA air concentration of about 0.006 mg/m<sup>3</sup>, assuming that the air concentration can be estimated from the soil concentration (1460 mg/kg) divided by the VF ( $3.8 \times 10^5$  m<sup>3</sup>/kg). In comparison, a no-effect level of 0.05 mg/m<sup>3</sup> has been estimated by extrapolation from toxicity data for GB (see Section 1.3.8). The soil trespasser PRGs for GA would therefore not be expected to result in an acutely toxic vapor concentration.

**Agent GD.** The maximum HBESL<sub>tres</sub> is 146 mg/kg for adolescent/adults. At this HBESL, the dose resulting from ingestion of 50 mg of soil is about 0.007 mg GD. A minimum effect level in humans is estimated to be 0.09 mg for oral exposures (see Section 1.3.8); therefore, the trespasser HBESL is expected to be marginally protective for acute toxicity resulting from ingestion of soil, for the stated conditions of exposure.

At the maximum HBESL<sub>tres</sub> of 146 mg GD/kg soil for adolescents/adults, and assuming a soil adherence of 0.08 mg per cm<sup>2</sup> of skin and a total exposed skin area of 5000 cm<sup>2</sup>, the total amount of soil on the skin would be 400 mg and would contain 0.05 mg of GD [146 mg/kg x (1 kg/1,000,000 mg) x 400 mg = 0.05 mg GD]. In comparison, it has been estimated that the minimum effect level for dermal exposures is 11 mg (see Section 1.3.8). Therefore, the trespasser HBESLs for GD are expected to be protective for acute dermal exposures for the stated conditions of exposure.

A soil HBESL of 146 mg/kg soil could theoretically result in a GD air concentration of 0.0009 mg/m<sup>3</sup>, assuming that the air concentration can be estimated from the soil concentration (146 mg/kg) divided by the VF ( $1.7 \times 10^5$  m<sup>3</sup>/kg). In comparison, a 1-hour no-effect level of 0.013 mg/m<sup>3</sup> has been estimated by extrapolation from toxicity data for GB (see Section 1.3.8); therefore, the soil HBESL<sub>tres</sub> would not be expected to result in acutely toxic vapor concentrations for the stated conditions of exposure.

**Lewisite.** The maximum calculated HBESL<sub>tres</sub> for Lewisite is 3650 mg/kg for adolescent/adults. At a soil HBESL of 3650 mg/kg, the dose resulting from ingestion of 50 mg of soil is 0.2 mg (0.003 mg/kg body weight). Estimates of MELs for orally administered Lewisite in laboratory animals range from 0.07 to 2

mg/kg (see Section 1.3.8). This is equivalent to dose range of 0.02 to 0.6 mg per animal. The  $HBESL_{tres}$  calculated using the RBC methodology may therefore not be protective for the stated conditions of exposure. To accommodate for potential acute effects the  $RBC_{tres}$  values were adjusted by a factor of 100 (see Table C-2). The resulting HBESLs of 27 and 36 mg/kg would correspond to an ingested dose of about 0.001 and 0.002 mg and would be expected to be marginally protective of acute oral toxicity.

In calculating the Lewisite PRGs for trespassers, a dermal RfD of 0.0000017 mg/kg was used (see Section 9.2 for derivation). The resulting  $HBESL_{tres}$  values are 66 mg/kg soil for adolescents and 76 mg/kg for adolescent/adults. At the HBESL of 76 mg/kg, and assuming a soil adherence of 0.08 mg per  $cm^2$  and a total exposed skin area of 5000  $cm^2$ , the total amount of soil on the skin would be 400 mg and would contain about 0.03 mg of Lewisite. The average concentration of Lewisite on the skin would be 0.000006 mg/ $cm^2$  (0.03 mg/5000  $cm^2$  = 0.000006 mg/ $cm^2$ ). Minimum effect levels (MELs) for percutaneous exposures to Lewisite were not found in the available literature. The median threshold dose for blistering was reported to be about 14  $\mu g$ , and a dose of 3.5  $\mu g$  resulted in erythema in 29 of 93 individuals and blistering in 8 of 93 (see Section 1.3.8). The MEL and no-effect level are likely to be below 1  $\mu g$ . The estimated percutaneous exposure at the HBESL of 76 mg/kg is 0.006  $\mu g/cm^2$ , therefore, the HBESLs are expected to be protective under the stated conditions of exposure.

A soil VF cannot be calculated for Lewisite because of its instability. Therefore, in the HBESL equation, the VF is replaced with the particulate emission factor ( $PEF = 1.32 \times 10^9$  m<sup>3</sup>/kg) to account for exposures through fugitive dust emissions. These HBESLs would also be appropriate for soil containing the nonvolatile breakdown products of Lewisite. A VF is available for one of the breakdown products, 2-chlorovinylarsonous acid (see Appendix I).

## C.6 CONCLUSIONS

As originally stated, though access to military installations is restricted, some instances of exposure of trespassers to residual chemical agent may occasionally occur. In most cases, these infrequent occurrences are not sufficient to warrant concern regarding a potential chronic risk. However, in those situations where there is a potential concern for repeated exposures to agent residues, the chronic exposures risk model and HBESLs<sub>tres</sub> described above may be a useful mechanism to determine if additional management/ engineering controls, treatment, or a more site-specific risk assessment are warranted.

This scenario demonstrates that the chronic risk assessment model may fail to accommodate the 'acute' risk from a single 'hotspot' of concentrated chemical agent. In situations where the calculated HBESL is at levels which approach potential acute toxicity concerns, it may be more prudent to consider the assessment of individual hotspots to ensure that the potential of acute risk is mitigated at these higher concentration levels. Only in situations where the agent is reasonably assumed to be homogeneously adsorbed or otherwise mixed in with the matrix (e.g., possibly waste soil or even more homogenous as in liquid matrices) is the use of the risk assessment model appropriate.



## APPENDIX D

### AGRICULTURAL/GRAZING SCENARIOS

The possibility exists that lands currently under the control of the Army will be leased for agricultural or grazing purposes. If chemical agent materials had at some time been disposed of on such lands, it would be necessary to certify that any residual amounts of material in the soil would be safe to the individuals involved in the above mentioned activities. The screening levels that would be appropriate for such uses would be dependent on several factors, the major one being whether any civilian populations actually resided on the land. In such cases residential Health-Based Environmental Screening Levels (HBESLs) could be used for such sites if appropriately modified to account for any unusual exposure routes or enhanced exposure through those exposure routes already addressed in the residential HBESLs.

**Ingestion of fruits and vegetables.** For example, one unique exposure route might be the ingestion of contaminated fruits or vegetables grown on the site. With the exception of sulfur mustard (HD), most of the chemical agents considered in this document have soil half-lives that are very short (see Table 2-3). Furthermore, the log  $K_{ow}$  values for the agents are relatively small (see Table 2-3) indicating a very low potential for bioaccumulation. Therefore, uptake of these agents into fruit or vegetables and/or the bioaccumulation through the food chain into farm animals is highly unlikely.

Although the potential for bioaccumulation of HD is low, bulk amounts of this agent can have a relatively long soil half-life when individual globules become encased by a oligomeric coating (formed with the hydrolysis products of HD) which prevents further dissolution and degradation. In this state encapsulated HD can remain in soil for many years, and the possibility exists that the agent may be released during farming operations. Under such circumstances, HD may be transferred into the air as vapors, or in windblown dust. Deposition on food crops is a theoretical, although very remote, possibility.

**Inhalation and dermal exposure.** As noted above, encapsulated HD can be sequestered in soil for many years. If the HD capsules are broken open, farm workers could be exposed through dermal contact, inadvertent soil ingestion, and inhalation of vapors or dust particulates. In such cases, the potential for acute exposures is much higher than in the scenarios used to establish the standard HBESL values. HBESLs cannot be established for such situations, and the necessary steps must be taken to ensure that HD is not present in encapsulated form.

**Ground water.** Because farm families may utilize well water as a source of drinking water, and because such water may not undergo standard water treatment procedures, ingestion of tapwater may be a very important exposure pathway for some types of contaminants. However, as discussed in Section 1.3.3 and Appendices E and H, the migration of chemical warfare agents through the soil to the underlining aquifer is considered to be highly unlikely. This is due primarily to the relatively rapid rates of degradation and/or to the immobility of the agent (as in the case of encapsulated HD). Because of their longer soil persistence times, and because they are generally more mobile in soils, the breakdown products of the chemical warfare agents are likely to have a greater potential for ground-water contamination than the agents themselves.

**Grazing.** The potential for long-term exposure to chemical agents on lands used for grazing is probably very low. As mentioned above, there is no evidence that any of the agents will bioaccumulate through the food chain. Furthermore the frequency, duration, and magnitude of exposure through dermal contact, inadvertent soil ingestion, and inhalation of vapors or particulates, is likely to be considerably less for ranchers than for farmers. The derivation of HBESLs for ranchers would be dependent on the selection of realistic values for the appropriate exposure parameters. It seems logical, however, that the HBESLs for ranchers would fall somewhere above those for trespassers and below those for industrial workers, and the use of the latter values would be a conservative approach.

## APPENDIX E

### MODELING POTENTIAL CHEMICAL AGENT CONTAMINATION OF GROUND WATER

#### E.1. OBJECTIVE

The general Army opinion is that chemical agents, because of their instability and volatility, will not remain in the environment long enough to contaminate ground water. The soundness of this opinion, however, has not until now been tested through the application of computer modeling to data.

The objective of this appendix is to model the potential for chemical agents to contaminate ground water in two generic climatic/geologic/contamination scenarios. The results will be in the form of horizontal distances from a site, beyond which any agents in ground water would be at or below predetermined evaluation endpoint concentrations (see Section E.4) .

#### E.2 CONCEPTUAL MODEL AND SOFTWARE USED

Chemical agent in soil will either volatilize into the air, adsorb onto organic soil constituents or dissolve into soil water. Infiltrating water passes by the agent, which dissolves (according to chemical-specific solubility factors) into liquid phase and travels vertically through the vadose (unsaturated) zone if field capacity is exceeded, until it reaches the water table (saturated zone). While traveling vertically, a portion of dissolved agent will continue to adsorb onto available organic material and volatilize into pore-air. This state of dynamic equilibrium is defined according to aspects of the infiltrating water, as well as chemical- and soil-specific characteristics. Upon reaching the water table, infiltrating water (or recharge) begins flowing generally horizontally along aquifer flow lines, transporting the remaining agent with it. While in liquid phase (i.e. while traveling vertically or horizontally), agent degrades through hydrolysis.

The software applied in this appendix includes a combination of VLEACH to model leaching from the vadose zone to ground water and a model developed by the U.S. Army Center For Health Promotion and Preventive Medicine (USACHPPM) for movement of the compounds after they enter the aquifer. VLEACH (Version 2.2a) is a one-dimensional finite difference vadose zone leaching model developed for the Robert S. Kerr Environmental Research Laboratory of the U.S. Environmental Protection Agency (USEPA) (Ravi and Johnson, 1996). It is based on the original VLEACH (version 1.0) developed for USEPA Region IX in 1990. The model estimates the impact on underlying ground water of the mobilization and migration of sorbed organic pollutants located in the vadose zone. VLEACH has been used to evaluate impacts of volatile organic contaminants at the Phoenix-Goodyear Airport Superfund site (Rosenbloom et al, 1993). Subsequently it has been used at numerous other sites. VLEACH and its documentation were obtained from

the website of the USEPA's Center for Subsurface Modeling Support (<http://earth1.epa.gov/ada/models.html>).

The second model, covering flow in the aquifer (i.e., horizontal flow), computes the amount of time required for a given concentration of chemical agent that reaches the vadose zone to hydrolyze to a specified concentration, in this instance the evaluation endpoint concentration for that agent (see Section E.4). This time is then multiplied by ground-water flow rate to calculate a horizontal distance from the source. Figure E-1 presents the equations used.

**Figure E-1:** Equations to compute time needed for compound to hydrolyze to evaluation endpoint concentration

If  $A(t)$  = amount of compound remaining at any time, then  $dA/dt = kA$ ,

	where:	
$k = \frac{-\ln 2}{t_{1/2}}$	$k$ = constant of proportionality	$t = \frac{-\ln FR}{k}$
	$t$ = time	
	$t_{1/2}$ = half-life	
	$FR$ = starting concentration/ endpoint concentration	

SOURCE: Zill, D.G., A First Course in Differential Equations, PWS-Kent Publishing, Boston, 1993

The chemical-specific parameters that were applied for the different chemicals in the VLEACH simulations are shown in Table E-1. Except for sulfur mustard (HD) and Lewisite, the hydrolysis half lives were taken from Table 1-1. The average hydrolysis rate is the geometric mean of all half-life values listed for each chemical. Table 1-1 listed a range for the hydrolysis half life of HD. The mean for HD, therefore is the arithmetic mean of the high and low values of the range presented, instead of the geometric mean of the three data points that were known. The fastest and slowest hydrolysis half-lives for HD are the lower and upper bounds of the listed range. Table 1-1 lists no estimate of the hydrolysis half-life for Lewisite. It states that the "solubility data are meaningless [for Lewisite] because of very rapid hydrolysis which is limited by rate of dissolution (Rosenblatt et al., 1975)." The average of 0.005 day assumed for Lewisite is thus highly conservative; the average rate, for example, is still larger than the fastest rate for HD, which, though fast, was slow enough to be measurable. The fastest and slowest hydrolysis rates for Lewisite are arbitrarily considered to be one order of magnitude higher and lower, respectively, than the average.

**Table E-1.** Chemical-specific parameters

Agent	Organic carbon distribution	Henry's constant	Water	Free air diffusion	Hydrolysis rates (half-lives in days)		
	coefficient (mL/g)	(dimensionless)	solubility (mg/L)	coefficient (m <sup>2</sup> /day)	Slowest	Average	Fastest
HD	133.0	0.00098	920	0.8554	0.0108	0.0067	0.0027
VX	327.0	0.00000033	30000	0.536	83.333	8.945	2.083
GB	34.6	0.000022	1090000	0.864	10.417	0.4186	0.02083
GA	38.5	0.00000623	98000	0.79488	0.3542	0.1563	0.0833
GD	234.0	0.000187	21000	0.70848	2.5	0.8664	0.0375
Lewisite	2.88	0.013	500	0.85536	0.05	0.005	0.0005

Because of its rapid hydrolysis, no estimate of the organic carbon distribution coefficient ( $K_{oc}$ ) could be calculated for Lewisite. Since several essential parameters are not available to derive  $K_{oc}$  for Lewisite, the only approach that seemed possible was to make a worst-case estimate. Accordingly, the  $K_{oc}$  was assumed to be one order of magnitude lower than the smallest  $K_{oc}$  of the other five chemicals. Because GB is miscible, the solubility was arbitrarily assumed to be  $1.09 \times 10^6$  mg/L, which is the same as its liquid density. Assuming a solubility of  $1.00 \times 10^6$  mg/L (as considered in another approach<sup>1</sup>) would yield only a slightly smaller estimate of GB's solubility in water. The choice was made to use the more conservative number.

### E.3 SCENARIO CHARACTERIZATIONS

Data from lithologic and hydrologic studies of the Edgewood Area of Aberdeen Proving Ground (USGS 1996) and the Tooele Army Depot (State of Utah, 1981; James M. Montgomery, 1987) were used to generate two generic landscape/climate scenarios. These were called the humid climate and arid climate scenarios, respectively. In addition to the landscape and rainfall parameters listed in Table E-2, the humid climate is defined as having a water table 3.7 meters (12 feet, per USGS 1996) below the ground surface, and the arid climate is defined as having a water table 59 meters (194 feet, per State of Utah 1981) below ground surface. Parameter values were chosen to correspond with a vadose zone comprised entirely of sand. This would tend to maximize agent transport and thereby produce a conservative estimate of ground-water contamination (for the purposes of risk assessment). The rates of flow (approximately horizontal) of ground water in the humid climate and arid climate scenarios were assumed to be 0.13 meter/day (per USGS 1996) and 1.22 meters/day (per James M. Montgomery, 1987), respectively.

<sup>1</sup> Small (1984) recommends solubility =  $1 \times 10^6$  mg/L if known to be infinitely soluble in water.

Hydrogeologic parameters such as depth to water table and ground-water flow rate can vary widely. Because of this, and to investigate the potential effects of individual parameters, the arid climate was also modeled with a water table depth of 3.7 meters (to demonstrate the effects of water table depth on an otherwise identical scenario), and again with the 3.7-meter depth and a ground-water flow rate of 0.13 meters/day. Both parameter values were taken from the humid climate. To further investigate the sensitivity of the agent VX in the arid scenario to soil organic carbon content and depth to water table, additional runs of the models were performed with varying levels of soil carbon and water table depth.

**Table E-2.** Landscape parameters used in VLEACH modeling

Parameter	Values used in humid scenario	Values used in arid scenario
recharge rate	0.46 meters/year	0.09 meters/year
dry bulk density	1.65 g/cm <sup>3</sup>	1.65 g/cm <sup>3</sup>
effective porosity	0.354	0.354
volumetric water content	0.177	0.09
saturation of soil	50%	25.4%
soil organic carbon content	0.0071	0.001
annual rainfall (used as one of several factors to estimate the recharge rate).	1.07 meters/year	0.55 meters/year

Documentation for VLEACH indicates that the fraction of organic matter in sand is 0.0071, which is used for the value in the humid climate. The organic content of the soil was assumed to be 0.001 for the arid climate to account for both a lower biologic activity (and therefore lower organic input to soil) and extreme depth to the water table (there generally being less organic matter at deeper depths) in arid regions.

In addition to the two landscapes modeled, the following two contamination scenarios were modeled; the “remediated” scenario and the “leak” scenario. In both cases, the top 1.22 meters (4 feet) of soil are uncontaminated, the next 0.61 meters (2 feet) of soil are contaminated, and the remainder of soil above the water table (57.3 meters or 1.83 meters for the arid climate, 1.83 meters for the humid climate) is uncontaminated at the start of the run of the model (i.e., at  $t_0$ ).

The remediated scenario is a hypothetical site of a past remediation project where any agents found will be at concentrations no higher than the HBESL for industrial sites, as listed in Table 11-2. The contaminated zone has an area of 92.9 square meters (1,000 square feet), and at  $t_0$  it is uniformly contaminated at the concentration listed as the industrial soil HBESL for each chemical (e.g., .85 mg VX/kg soil). There are, therefore, 56.7 m<sup>3</sup> of soil that are uniformly contaminated. It is assumed that the entire quantity of agent seeping into the ground water on a given day dissolves into 1000 L of water at the exact

starting point for application of the horizontal flow model. Because hydrolysis is occurring as ground water moves across the water table directly beneath the contaminated zone of 1000 ft<sup>2</sup>, this method should greatly overestimate the true concentration at the starting point for the horizontal-flow model.

In the simulated leak, the contaminated zone has an area of 0.09 square meters (1 square foot), and at  $t_0$  it is uniformly contaminated with 500,000 mg of chemical per kg of dry soil. There are, therefore, 0.06 m<sup>3</sup> (2 ft<sup>3</sup>) of soil uniformly contaminated. It is assumed that the entire quantity of agent seeping into the ground water on a given day dissolves into 1 L of water. If a buried chemical munition would suddenly start to leak, it would likely take many days for equilibrium to be reached at 500,000 mg/kg. Simultaneous hydrolytic degradation would further slow, and possibly deny, attainment of equilibrium. Thus, the described situation will likely considerably overestimate the possible agent source.

#### E.4 DERIVING AN EVALUATION ENDPOINT

It is necessary to define for the modeling a non-zero, positive concentration value that describes a 'no-risk' level of agent. For those situations where an open drinking water source is initially contaminated (either through accidental or intentional release), initial evaluation of the associated risks may involve comparison with the Army's Field Drinking Water Standards (FDWS) (DA 1996b). These values were derived to ensure adequate protection of a healthy male military population consuming 5-15 L of water per day for up to 7 days. While the soldier consumption rate is significantly larger than the USEPA assumption of 2 L/day for the general civilian population, individuals within the civilian population (such as elderly and children) may be somewhat more susceptible to agent toxicity than the military population, and the USEPA default assumption for exposure duration is much longer (30 years). Therefore, to ensure an extremely conservative evaluation, the worst case assumption of potential long-term contamination of a general population water supply was used in determining agent concentration endpoints for the model.

##### E.4.1 Method of Derivation

The EPA Region IX PRG risk assessment methodology for tapwater (USEPA, 1996b) can be used to calculate evaluation endpoint concentrations for the chemical agents. These extremely conservative values can then be used to simulate an extreme worst case agent migration scenario. The Region IX method includes potential exposure by two pathways: ingestion of drinking water and inhalation of volatiles that might be released from tapwater during routine household activities.

For noncarcinogenic endpoints, the algorithm used for calculating an evaluation endpoint for ground-water modeling is as follows:

$$PRG_{dw} = \frac{THQ \times BW \times AT_n \times 1000 \text{ ug/mg}}{EF \times ED \times \left( \frac{IRW}{RfD_o} + \frac{VF_w \times IRA}{RfD_i} \right)}$$

For contaminants having a carcinogenic effect, the algorithm used for calculating an evaluation endpoint for ground-water modeling is as follows:

$$PRG_{dw} = \frac{TR \times AT_c \times 1000 \text{ ug/mg}}{EF [ (VF_w \times InhF_{adj} \times CSF_i) + (IFW_{adj} \times CSF_o) ]}$$

The values of several of the listed parameters, including the toxicity values (reference doses (RfDs) and cancer slope factors (CSFs)), averaging times for carcinogenic and noncarcinogenic effects ( $AT_c$  and  $AT_n$ ), body weight (BW), exposure duration (ED), and inhalation rate (IRA), are the same as those used in the HBESL calculations for residential scenarios presented elsewhere in this document. Other exposure parameters are more specific to the tapwater scenario as described by EPA Region IX guidance. The unique additional exposure assumptions used to calculate values for the agents are presented below.

**Volatilization Factor (VF).** Health risks associated with inhalation of chemicals indoors are relevant only for chemicals that easily volatilize from water during household activities such as showering, laundering, and dish washing. The PRG screening levels for tapwater incorporate a volatilization factor ( $VF_w$ ) that is applicable only to volatile chemicals. According to EPA criteria, only sulfur mustard is considered volatile (please see Sec. 1.3.6 for a more detailed discussion of EPA criteria for defining volatility). It should be noted, however, that hydrolysis of HD is very rapid (half-life 0.08 hr), and trace amounts of HD would not be stable in water. Therefore, volatilization from water (and therefore the inhalation pathway) is not likely to be significant.

The USEPA criterion for volatility is used only to identify those chemicals for which the inhalation pathway should be considered when deriving PRGs (USEPA, 1991a). USEPA (1991a) reported that the experimental data of Andelman (1990), which defined the relationship between the concentration of a chemical in tapwater and its concentration in indoor air (based on data for radon), included a default volatilization constant of 0.5 L/m<sup>3</sup>. This is the volatilization factor that is used to derive PRGs for tapwater.

**Inhalation rate and age-adjusted inhalation factor ( $IRA$ ,  $InhF_{adj}$ ).** As noted above, the inhalation pathway is not expected to be a significant source of exposure for any of the agents based on their Henry's Law Constants or rapid rate of very rapid hydrolysis (agent HD). Therefore, the inhalation pathway is not included in the calculations for evaluation endpoints.

**Ingestion of tapwater and tapwater-based drinks (IRW).** For the tapwater exposure pathway, the standard USEPA default for drinking water consumption is 2 L/day for adults. An intake rate of 2 L/day is considered a maximum value (approximately the 90<sup>th</sup> percentile), and 1.4 L/day is considered a reasonable estimate of the average daily intake (USEPA, 1989a). USEPA currently uses 1 L/day as the default value for children. For ingestion of tapwater and water-based drinks, USEPA estimated that 75 to 100% of such intake would occur at the place of residence (USEPA, 1989a). For calculating screening levels, the conservative assumption is made that consumption of tapwater and water-based drinks occurs entirely at the place of residence.



### E.4.2 Derivation Results

The calculated evaluation endpoint values to be used in modeling in this appendix include: 0.087  $\mu\text{g/L}$  for HD (based on cancer risk level of  $10^{-5}$ ); 0.022 for  $\mu\text{g/L}$  GA; 0.73 for  $\mu\text{g/L}$  GB; 1.5  $\mu\text{g/L}$  for GD; and 0.15  $\mu\text{g/L}$  for VX; and 3.7  $\mu\text{g/L}$  for Lewisite.

## E.5 RUNNING THE MODELS

Model runs were performed on each agent individually, in all climate/scenario combinations (arid remediated, arid leak, humid remediated, humid leak) at each rate of hydrolysis (fastest, average, and slowest), for a total of 12 runs per agent. Additional runs were performed with an altered arid climate, for all scenarios and hydrolysis rates, totaling an additional 12 runs per agent. Also, as mentioned earlier, 5 additional runs were performed on an altered arid climate “leak” scenario for agent VX, varying soil carbon and depth to ground water.

VLEACH modeled the movement of contamination (incorporating adsorption but not considering hydrolysis) and estimated the number of grams of chemical reaching the water table on each ensuing day. This concentration was then put through independent calculations of exponential decay to determine how much agent, minus the portion hydrolyzed during vertical flow, actually enters ground water. The output from a complete run of VLEACH is too large to include in this appendix; however, complete copies are available upon request. Table E-3 lists the concentrations of agents predicted to reach the water table, broken out by agent, climate (arid/humid), scenario (remediated/leak), and hydrolysis rate. This concentration is used as the starting concentration in the horizontal-flow model. As mentioned above, the second model generates the time necessary to degrade a given concentration of agent to a specified level (the evaluation endpoint concentration for that agent), then combines this time with ground-water flow velocity to calculate a distance. Figure E-2 presents an example run of the horizontal-flow model. Table E-4 lists the horizontal distances away from the contamination site that ground water will travel before dissolved agent concentrations will fall below evaluation endpoint levels, broken out by agent, climate (arid/humid), scenario (remediated/leak), and hydrolysis rate.

**Figure E-2:** Example run of the horizontal-flow model

The humid climate, leak scenario of GD lists an actual concentration of  $1.69\text{E}+1 \mu\text{g/L}$  reaching ground water (see Table E-3). Table E-1 lists an average hydrolysis half-life for GD of 0.8664 days, and Section H.4.2 lists an evaluation endpoint level of  $0.15 \mu\text{g/L}$  for GD. Therefore:

$$k = -\ln 2 / 0.8664 = -0.80003$$

$$\text{starting concentration/evaluation endpoint} = (1.69 \times 10^1) / 0.15 = 1.13 \times 10^2$$

$$t = -\ln(1.13 \times 10^2) / 0.80003 = 5.91 \text{ days}$$

$$\text{Then, } (5.91 \text{ days})(0.13 \text{ meters/day}) = 0.756 \text{ meters}$$

Therefore, when ground water contaminated with the agent GD has traveled approximately 0.76 meters from the point where contamination entered ground water, concentrations of GD will be at or below evaluation endpoint levels.

Table E-3. Maximum concentrations of chemical agent reaching water table (Unless otherwise noted, maximum concentrations arrived on day one.)				
Agent	Scenario	Concentration (μg/L)		
		(Slowest Hydrol. Rate)	(Avg. Hydrol. Rate)	(Fastest Hydrol. Rate)
Arid Climate - deep water table				
HD	remediated <sup>b</sup>	2.45E-51	1.13E-68	1.27E-134
	leak <sup>b</sup>	5.11E-48	2.36E-65	2.65E-131
VX	remediated <sup>b</sup>	9.92E-33	9.26E-33	7.17E-33
	leak <sup>b</sup>	5.84E-30	5.45E-30	4.22E-30
GB	remediated <sup>b</sup>	9.56E-23	1.95E-23	3.61E-37
	leak <sup>b</sup>	1.84E-21	3.75E-22	6.94E-36
GA	remediated <sup>b</sup>	6.99E-25	5.87E-26	1.20E-27
	leak <sup>b</sup>	8.13E-24	6.83E-25	1.40E-26
GD	remediated <sup>b</sup>	1.76E-25	1.04E-25	2.18E-33
	leak <sup>b</sup>	1.69E-23	1.00E-23	2.10E-31
L <sup>a</sup>	remediated <sup>b</sup>	4.33E-25	2.83E-79	<1E-300
	leak <sup>b</sup>	1.27E-24	8.31E-79	<1E-300
Humid Climate - shallow water table				
HD	remediated <sup>b</sup>	3.80E-30	1.75E-47	1.97E-113
	leak <sup>b</sup>	7.91E-27	3.65E-44	4.10E-110
VX	remediated <sup>b</sup>	5.27E-6	4.92E-6	3.81E-6
	leak <sup>b</sup>	3.10E-3	2.89E-3	2.24E-3
GB	remediated <sup>b</sup>	1.64E-2	3.34E-3	6.18E-17
	leak <sup>b</sup>	3.14E0	6.42E-1	1.19E-14
GA	remediated <sup>b</sup>	9.38E-3	7.87E-4	1.62E-5
	leak <sup>b</sup>	1.09E-1	9.15E-3	1.88E-4
GD	remediated <sup>b</sup>	3.23E-2	1.92E-2	4.01E-10
	leak <sup>b</sup>	3.11E0	1.84E0	3.85E-8
L <sup>a</sup>	remediated <sup>b</sup>	1.73E-3	1.13E-57	<1E-300
	leak <sup>b</sup>	5.10E-3	3.33E-57	<1E-300
Arid Climate - shallow water table				
HD	remediated <sup>b</sup>	1.01E-28	4.66E-46	5.24E-112
	leak <sup>b</sup>	2.10E-25	9.70E-43	1.09E-108
VX	remediated <sup>b</sup>	2.22E-4	2.07E-4	1.60E-4
	leak <sup>b</sup>	1.30E-1	1.22E-1	9.43E-2
GB	remediated <sup>b</sup>	3.05E0	6.23E-1	1.15E-14
	leak <sup>b</sup>	5.87E+1	1.20E+1	2.22E-13
GA	remediated <sup>b</sup>	1.91E-1	1.60E-2	3.29E-4
	leak <sup>b</sup>	2.22E0	1.86E-1	3.82E-3
GD	remediated <sup>b</sup>	1.07E0	6.32E-1	1.32E-8
	leak <sup>b</sup>	1.03E+2	6.08E+1	1.27E-6
L <sup>a</sup>	remediated <sup>b</sup>	1.78E-2	1.16E-56	<1E-300
	leak <sup>b</sup>	5.25E-2	3.42E-56	<1E-300

a Values for Lewisite may be extreme overestimates as discussed in text.

b See section E.3 - SCENARIO CHARACTERIZATIONS for definitions of the "remediated" and "leak" scenarios.

Table E-4. Predictions of ground-water flow before complete hydrolysis <sup>a</sup> of chemical agent				
Agent	Scenario	Horizontal distance (m) from site of contamination		
		(Slowest Hydrol. Rate)	(Avg. Hydrol. Rate)	(Fastest Hydrol. Rate)
Arid Climate - deep water table				
HD	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
VX	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
GB	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
GA	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
GD	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
L	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
Humid Climate - shallow water table				
HD	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
VX	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
GB	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	2.9	0	0
GA	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
GD	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	1.4	0.4	0
L	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
Arid Climate - shallow water table <sup>c</sup>				
HD	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0
VX	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	260.6	27.0	5.3
GB	remediated <sup>b</sup>	26.2	0	0
	leak <sup>b</sup>	80.4	2.1	0
GA	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0.2	0	0
GD	remediated <sup>b</sup>	8.6	2.2	0
	leak <sup>b</sup>	28.7	9.2	0
L	remediated <sup>b</sup>	0	0	0
	leak <sup>b</sup>	0	0	0

a "Complete hydrolysis" defined as the evaluation endpoint levels calculated in section H.4.

b See section E.3 - SCENARIO CHARACTERIZATIONS for definitions of the "remediated" and "leak" scenarios.

c Original ground-water flow rate (1.22 m/day) used. Altered flow rate (0.13 m/day) used in Table E-5.

The arid climate was further altered to reflect both the water table depth and ground-water flow rates

of the humid climate, so that comparisons could be made. Table E-5 shows this comparison. The slight differences- 1.4 m (humid) vs. 3.1 m (arid) found in the GD “leak” scenario for example- may be due to the greater soil organic carbon content found in the humid soil. With more organic carbon on which to adsorb, less agent will travel.

<b>Table E-5.</b> Comparison of humid and arid climates with the same depth to water table and ground-water flow rate  Distances ground water travels before chemicals hydrolyze to below evaluation endpoint levels							
Agent	Scenario	Horizontal distance (m) from site of contamination					
		(Slowest Hydrol. Rate)		(Avg. Hydrol. Rate)		(Fastest Hydrol. Rate)	
		Humid	Arid	Humid	Arid	Humid	Arid
HD	remediated <sup>a</sup>	0	0	0	0	0	0
	leak <sup>a</sup>	0	0	0	0	0	0
VX	remediated <sup>a</sup>	0	0	0	0	0	0
	leak <sup>a</sup>	0	27.8	0	2.9	0	0.6
GB	remediated <sup>a</sup>	0	2.8	0	0	0	0
	leak <sup>a</sup>	2.9	8.6	0	0.2	0	0
GA	remediated <sup>a</sup>	0	0	0	0	0	0
	leak <sup>a</sup>	0	0	0	0	0	0
GD	remediated <sup>a</sup>	0	0.9	0	0.2	0	0
	leak <sup>a</sup>	1.4	3.1	0.4	1.0	0	0
L <sup>a</sup>	remediated <sup>a</sup>	0	0	0	0	0	0
	leak <sup>a</sup>	0	0	0	0	0	0

a See section E.3 - SCENARIO CHARACTERIZATIONS for definitions of the “remediated” and “leak” scenarios.

To further investigate the potential of both soil carbon and depth to water table to effect final output, additional runs of the models were performed using the agent VX/arid/leak combination. Table E-6 shows the outcomes, detailing parameter values used and the horizontal distance traveled by aqueous agent before hydrolyzing to below evaluation endpoint levels. According to these models, VX is clearly highly sensitive to organic carbon content in the soil. This is not surprising, considering VX has the highest  $K_{oc}$  (i.e., the highest affinity to organic carbon) of any of the agents modeled. It is also clear that the vertical distance these compounds must travel before reaching ground water has a substantial effect.

<b>Table E-6.</b> Effects of soil carbon and water table depth on horizontal distance traveled		
Agent VX, arid climate, leak scenario, 1.22 m/day flow rate, slowest hydrol. rate		
Organic Carbon Content	Depth to Water Table (m)	Horiz. Distance Traveled (m)
0.001*	3.7*	260.6*
0.002	3.7	170.2
0.003	3.7	114.4
0.0035	3.7	93.1
0.001	4.9 (16 feet)	47.0
0.002	4.3 (14 feet)	63.4

\* from Table E-4

## E.6 DISCUSSION AND CONCLUSIONS

The following points were considered during the development and use of these models:

Karst and macropore formations - Vadose water and ground water can be modeled in karsts and macropore formations, but only with great difficulty and uncertainty. The models used in this appendix do not apply to karsts and macropores.

Multiple soil types - It is reasonable (and only practical, without investment of much more effort) to assume that there is a single soil type of moderately high hydraulic conductivity rather than attempting to estimate the combined effects of bands of different soil types having different thicknesses. Such an assumption is likely to lead to an overestimation of the rate at which substances pass through the vadose zone. Also, a single-soil value is more "generic" than a multi-soil value. It should be understood that the values generated for this appendix are only valid for homogeneous subsurface conditions.

Diffusion - An assumption that there is no diffusion adds conservatism to the outcome by increasing agent concentration.

Evapotranspiration - An assumption that there is no evapotranspiration adds conservatism by increasing the volume of agent reaching ground water.

Soil pH - Chemical agent hydrolysis rates are often highly pH dependent (see Table 1-1), but disagreement is found in the literature. Some of the slowest and fastest hydrolysis rates considered occur at pH's unlikely to be encountered in nature. Further research should be conducted into the correlation between soil pH and chemical agent hydrolysis rates.

Choices regarding models and parameter values used, and assumptions made, among other choices, were influenced by the intent to generate estimates of concentration and distance that would be reasonably, but not overly, conservative. The intent was not to characterize an actual scenario as completely as possible, but rather to calculate worst-case values for a range of possible sites/scenarios, which actual values would be unlikely to exceed.

As noted above, horizontal distances required to reach evaluation endpoint levels are zero for the great majority of all scenarios. In most cases, dissolved chemical agent migrating vertically through the vadose zone hydrolyzes to below endpoint levels before ever reaching ground water. Of those predicted to have some horizontal flow, only one shows a distance over 100 meters. Considering the level of conservatism incorporated in the modeling, the results tend to support the view that the chemical agents modeled are not likely to contaminate ground water. Future modeling efforts should consider the following:

Particularly in situations of limited precipitation (e.g., arid climates or drought conditions), evapotranspiration is an important parameter to include in fully characterizing potential groundwater contamination. A percentage of precipitation will evaporate from the surface or be transpired by local plant life. This percentage is then no longer available to transport chemical agent to the water table. At the extreme at which all precipitation evapotranspires, there is none available for agent transport. In effect, the pathway is broken before the agent reaches groundwater and, hence, the agent does not pose a threat to receptors via ground water. This is not an unreasonable scenario: In the Tooele region of Utah, for instance, local precipitation does not contribute to groundwater; all recharge comes from the surrounding mountains. Since there has been no opportunity yet to explicitly model evapotranspiration, this is one area in which additional modeling could reduce the level of uncertainty associated with model output.

Geologic and hydrologic conditions such as soil type, depth to water table, and hydraulic conductivity can vary widely at any individual site. This makes developing “generic” distance-from-site numbers of any sort difficult and “universal” numbers (equally valid in any scenario) unlikely. Also, failure to fully characterize site-specific hydrogeology for any site increases the uncertainty associated with model output.

Perhaps due to their military-unique nature, comparatively little research has been performed on these chemical agents, as opposed to hazardous chemicals used in industry. There is considerable disagreement in the literature on a number of chemical-specific parameters (as the range of values for hydrolysis rates will attest), and there are still many data gaps (hydrolysis and  $K_{oc}$  values for Lewisite, for example). Larger data gaps exist regarding the fate and transport of chemical agents in the environment. Available hydrolysis rates for agents are based on pure agent dissolved in various volumes of unbuffered water, rather than agent found in soil, where the available data suggest hydrolysis is considerably faster.

Even less is known about the degradation products of chemical agents (see Appendix F). Several of these products, particularly EA-2192 and Lewisite oxide/chlorvinyl arsonous acid (CVAA), are estimated to be somewhat more environmentally stable than the source agents, while are assumed to retain significant toxic properties. Since this particular assessment does not address the potential for these breakdown /degradation products to migrate via groundwater, further research to determine the environmental parameters for these compounds, as well as modeling their potential for ground-water contamination, may be warranted.

Model calibration (i.e., multiple runs during which variable parameters are altered until output consistently matches empirical evidence) is a vital step in ensuring that any predictions made by the model can be considered valid. Unfortunately, a very limited database was available to calibrate these models<sup>2</sup>. In addition to the fate and transport research mentioned above, additional research is needed to develop empirical evidence against which future modeling can be verified.

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<sup>2</sup> Other reports regarding the USGS study of New O-field at the Edgewood Area of APG reported that no chemical agents that were tested for were found in ground water, which agrees with predictions made using the models discussed in this appendix.



## APPENDIX F

## PRIMARY BREAKDOWN PRODUCTS OF CHEMICAL AGENTS

The breakdown products of the chemical agents discussed in this report that are considered to be relatively persistent in the environment and/or potentially toxic are listed in Table F-1. These compounds were identified through an assessment of various breakdown products formed through different processes (Munro et al., submitted for publication, Dec 1998).

Table F-1. Primary chemical agent degradation products of potential concern in the environment				
Agent	Degradation Product	Formula	CAS No.	Chronic Toxicity Values <sup>a</sup>
<b>Sulfur Mustard (HD)</b>	Thiodiglycol (TDG)	C <sub>4</sub> H <sub>10</sub> SO <sub>4</sub>	111-48-8	RfD <sub>o</sub> = 0.17 mg/kg/day <sup>b</sup>
<b>Tabun (GA)</b>	None of potential concern	-	-	-
<b>Sarin (GB)</b>	Methyl phosphonic acid (MPA)	CH <sub>3</sub> PO <sub>3</sub>	993-13-5	RfD <sub>o</sub> = 0.02 mg/kg/day <sup>b</sup>
	Isopropyl methylphosphonic acid (IMPA)	C <sub>4</sub> H <sub>11</sub> PO <sub>3</sub>	1832-54-8	RfD <sub>o</sub> = 0.10 mg/kg/day
<b>Soman (GD)</b>	Methyl phosphonic acid (MPA)	CH <sub>3</sub> PO <sub>3</sub>	993-13-5	RfD <sub>o</sub> = 0.02 mg/kg/day <sup>b</sup>
<b>Agent VX</b>	S-(Diisopropylaminoethyl) methylphosphonothioate (EA-2192)	C <sub>9</sub> H <sub>22</sub> NSPO <sub>2</sub>	73207-98-4	RfD <sub>o</sub> = 6 x 10 <sup>-7</sup> mg/kg/day <sup>c</sup>
	Ethyl methylphosphonic acid (EMPA)	C <sub>3</sub> H <sub>9</sub> PO <sub>3</sub>	1832-53-7	RfD <sub>o</sub> = 0.028 mg/kg/day <sup>c</sup>
	Methyl phosphonic acid (MPA)	CH <sub>3</sub> PO <sub>3</sub>	993-13-5	RfD <sub>o</sub> = 0.02 mg/kg/day <sup>b</sup>
<b>Lewisite</b>	2-chlorovinyl arsonous acid (CVAA) <sup>h</sup>	C <sub>2</sub> H <sub>4</sub> AsClO <sub>2</sub>	85090-33-1	RfD <sub>o</sub> = 0.0001 mg/kg/day <sup>f</sup>
	Lewisite oxide (Chlorovinyl arsenous oxide <sup>g</sup> )	C <sub>2</sub> H <sub>2</sub> ClAsO	3088-37-7	RfD <sub>o</sub> = 0.0001 mg/kg/day <sup>f</sup>
	Vinyl chloride	C <sub>2</sub> H <sub>3</sub> Cl	75-01-4	-
	Inorganic arsenic <sup>i</sup>	As	7440-38-2	RfD <sub>o</sub> = 0.3 µg/kg/day <sup>d</sup> ; oral SF <sup>d</sup> = 1.5 (mg/kg/day) <sup>-1</sup> ; inhalation unit risk <sup>d</sup> = 0.0043 per µg/m <sup>3</sup>

<sup>a</sup> Toxicity values developed by USACHPPM (see Annex F.1) unless otherwise indicated

<sup>b</sup> QSAR estimate.

<sup>c</sup> Based on similar toxic properties of the related compound isopropyl methyl phosphonic acid (RfD = 0.2 mg/kg; EPA, 1997a)

<sup>d</sup> EPA 1997a, *Integrated Risk Information System (IRIS)*. Online file.

<sup>e</sup> RfD is the same as that used for VX

<sup>f</sup> RfD is the same as that used for Lewisite

<sup>g</sup> Also referred to as Lewisite oxide, is a dehydration product of Lewisite; it is assumed that in most ambient environments Lewisite oxide would immediately replace its parent compound

<sup>h</sup> 2-chlorovinyl arsonous acid (CVAA) is more likely to be found in aqueous matrices than Lewisite or Lewisite oxide. However, since CVAA is of limited persistence and in many cases has limited solubility, it may not be a significant concern for contamination of aqueous media such as groundwater. Instead, inorganic arsenic should be evaluated in cases where Lewisite contamination is suspected.

<sup>i</sup> As arsenic is ubiquitous in the environment and may be present in significant concentrations from sources having no relationship to agent, evaluations of arsenic must be done with adequate data on background arsenic concentrations. See text.

The compounds in Table F-1 may be useful as "indicators" of past chemical agent presence but, in addition, there may be some questions as to the potential health risks associated with these breakdown/degradation products in certain environmental scenarios. The risk assessment methodologies described throughout this report can be used to determine Health Based Environmental Screening Levels (HBESLs) for some of the potential toxic compounds. The risk assessment algorithms require the input of chronic toxicity values (e.g., RfD<sub>s</sub> and for noncarcinogens and CSF<sub>s</sub> for carcinogens). The USEPA approved chronic toxicity values are available for only a few of these compounds. Where EPA values were not available, they were estimated by USACHPPM using Quantitative Structure-Activity Relationships (QSAR) methods or by comparison with structurally related compounds (see Table F-1 and also Annex F.1). These toxicity values have not yet been verified by EPA. The values presented are based on currently available data with certain extrapolations or assumptions, and are only presented as suggested values pending further study and review. For those breakdown compounds deemed of significant toxicity, example screening levels have been calculated using methods and described previously in this document.

The information below summarizes the basis for selected the identified compounds in Table F-1 as described in Munro et al, submitted for review, December 1998. Toxicity estimates are based on the derivations described in Annex F.1

**Agent HD.** When dissolved in water agent HD hydrolyzes rapidly to thiodiglycol. Thiodiglycol (TDG) has a high RfD (0.17 mg/kg/day), indicating that it is relatively nontoxic; therefore, HBESLs have not been calculated for it. Its presence in soil or water can be used as an indicator of past contamination with agent HD, although it is not unique to HD degradation due to the possible commercial application of thiodiglycol in the manufacture of soap products and polymers. Other, secondary degradation products may be found in certain soil types. In particular, the compound thiodiglycolic acid (TDGA) may occur through a biological transformation of TDG, though this may not occur in all soil types.

**Agent GA.** As described previously in this document (Section 1.2.3), Agent GA is not persistent in the environment. Literature reviews have not established any environmentally persistent or toxic degradation products that would be associated with this agent.

**Agent GB.** Methyl phosphonic acid (MPA) is the primary breakdown product of agent GB. The estimated oral RfD is 0.02 mg/kg/day, indicating that it is relatively nontoxic; therefore, HBESLs were not calculated. A secondary breakdown product of Agent GB is isopropyl methylphosphonic acid (IMPA), with an estimated RfD of 0.1 mg/kg/day (relatively nontoxic). As a consequence, no HBESLs were calculated for this compound.

**Agent GD.** Methyl phosphonic acid (MPA) is the primary breakdown product of agent GD. The estimated oral RfD is 0.02 mg/kg/day, indicating that it is relatively nontoxic; therefore, HBESLs were not calculated.

**Agent VX.** Agent VX has three primary breakdown products, EA-2192, ethyl methylphosphonic acid (EMPA) and methyl phosphonic acid (MPA). EA-2192 has an estimated vapor pressure of  $5.24 \times 10^{-6}$  mm Hg, an estimated water solubility of  $1.4 \times 10^4$  mg/L at 25°C, an estimated  $K_{ow}$  of 1.52, and an estimated

Henry's Law Constant of  $4.38 \times 10^{-12}$  atm-m<sup>3</sup>/mol (Howard and Meylan, 1997). According to the USEPA, compounds with Henry's Law Constants less than  $1 \times 10^{-5}$  atm-m<sup>3</sup>/mol are not likely to pose an inhalation hazard as a result of volatilization from water or soil. Because of its relatively high water solubility, EA-2192 is a potential contaminant of groundwater. The estimated oral RfD for EA-2192 was set at the same value as the RfD for VX (see Annex F.1). This is believed to be an extremely conservative approach because EA-2192 exists in an ionized state which would reduce absorption through the gastrointestinal tract. In addition, acute oral and dermal toxicity data indicate that EA-2192 is somewhat less toxic than VX by these pathways (see Annex F.2). However, given the paucity of data and various uncertainties, the conservative approach is suggested. HBESLs for EA-2192 are listed in Table F-2.

The estimated oral RfD for EMPA is 0.03 mg/kg/day and that for MPA is 0.02 mg/kg/day. Therefore, both of these breakdown products are considered to be relatively nontoxic and HBESLs were not calculated for them.

**Lewisite.** In aqueous media, Lewisite hydrolyzes to 2-chlorovinyl arsonous acid (CVAA). In an aqueous solution (to include soil with significant moisture) the primary Lewisite degradation product present expected is 2-chlorovinyl arsonous acid; Lewisite oxide (also referred to as chlorovinyl arsenous oxide or chlorovinyl arsenoxide) occurs only as a dehydration reaction products and therefore maybe expected in drier media. Given the limited data available, CVAA and Lewisite oxide are currently considered to be as toxic as Lewisite itself. HBESLs for 2-chlorovinyl arsonous acid/Lewisite oxide are listed in Table F.2. However, it should be noted that both CVAA/Lewisite oxide will further degrade resulting in the formation of vinyl chloride and inorganic arsenic. *These compounds, particularly inorganic arsenic, should be considered the primary constituent of concern when evaluating environmental media for potential Lewisite contamination - its is particularly unlikely that the other compounds would persist long enough to present a chronic health risk.*

It is important to realize, however, that in evaluating sites for arsenic contamination as a potential result from Lewisite degradation, consideration must be given to naturally occurring background levels of arsenic - arsenic is ubiquitous in environmental media and in many geographic areas may be found in concentrations greatly exceeding health/risk - based screening levels. Specifically, national background concentrations range from about 1 - 40 ppm, with a mean value of about 5 ppm; however, soils overlying arsenic rich ores may have concentrations two orders of magnitude higher. In addition, industry (e.g. smelter operation) and agricultural applications (pesticides/herbicides) may retain substantial amounts of arsenic (ATSDR, 1993). In addition, the valence state of the arsenic present at a site must be determined. This is important because the toxicity of inorganic arsenic varies with valence state, with the trivalent form being much more toxic than the pentavalent form. Environmental screening levels (e.g. PRGs) for vinyl chloride and inorganic arsenic are available from EPA Region IX (USEPA, 1996b/1998) and are therefore not calculated in this document but should be considered when evaluating media/sites for Lewisite contamination.

<b>Table F-2. Summary of calculated HBESLs for key agent breakdown products</b>
---------------------------------------------------------------------------------

	Residential soil (mg/kg)			Industrial soil (mg/kg)		
	RBCs	PRGs	SSLs	RBCs	PRGs	SSLs
<b>EA-2192</b> <sup>a</sup>	0.047	0.042	0.047	1.2	1.1	NA
<b>2-Chlorovinyl- arsonous acid/Lewisite oxide</b> <sup>b</sup>	7.8	0.3	7.8	(7.8) <sup>c</sup>	3.7	NA

<sup>a</sup> Based on VX toxicity; parallels VX screening levels

<sup>b</sup> These values are based on Lewisite toxicity; In addition, vinyl chloride and arsenic should be evaluated during site assessments. The existing USEPA screening levels for these two compounds should be consulted.

<sup>c</sup> As with Lewisite calculations, RBC value derived for the commercial/industrial scenario was potentially above acute toxicity levels, therefore the upper bound value of the residential scenario is suggested as a substitute. See Section 9.1 of this document.

**Summary.** When evaluating chemical agent contamination in environmental media, it is necessary to realize that under many if not most circumstances, the agent will breakdown/degrade in relatively short amounts of time. While analyses may not show the presence of agent, there may be a need to determine previous presence of agent or, in certain circumstances, there may be a breakdown product that itself poses a potential health risk of concern. Though there are numerous breakdown products, only a few are substantially persistent in the environment and even fewer that are of significant toxicity. Specifically, the products EA-2192 (from VX) and CVAA and Lewisite oxide from Lewisite are potential health concerns and may need to be evaluated against HBESLs or through a site-specific health risk assessment. Also, inorganic arsenic should be evaluated at sites involving Lewisite, though care must be given to proper evaluation of naturally occurring/anthropogenic background concentrations of arsenic (this compound is currently regulated and there are existing EPA screening levels). Other persistent compounds of relatively insignificant toxicity include TDG (from HD), and MPA and EMPA (from VX and GB and GD) which may be useful in tracing previous agent presence or sources. Finally, the assessor should be aware of other potential contaminants associated with the source of chemical agent such as chloroform from Chemical Agent Identification Sets (CAIS) for which there are also existing EPA screening levels.

**APPENDIX F - ANNEX F.1**

MCHB-TS-THE

10 December 1998

MEMORANDUM FOR: Veronique Hauschild, Chemical Agent Systems Working Group,  
USACHPPM, Aberdeen Proving Ground, MD 21010

SUBJECT: Report on Suggested RfD and RfC for Selected Agent-Related Compounds

1. Attached is a report entitled "Suggested Interim Estimates of the Reference Dose (RfD) and Reference Concentration (RfC) for Certain Key Breakdown Products of Chemical Agents"
2. These estimates are only interim in nature and are intended to assist with risk assessments of chemical agent contaminated sites. The compounds dealt with may have to be sampled for in soil, water or air for purposes of human health and ecological risk assessment. The estimates will be of use in making cleanup decisions regarding polluted sites or following spill events. They will also be of use in developing safe processes for demilitarization/detoxification of agents and agent-containing munitions.
3. In developing the estimates, existing values for the RfD were first ascertained. If there were none, proposed RfDs, developed from experimentally-determined NOAELs or LOAELs were considered. If there were none, then a RfD estimate was estimated using (1) a NOAEL or LOAEL determined for a structurally-related compound or (2) a rat chronic LOAEL estimated by Quantitative Structure-Activity Relationships (QSAR). The QSAR system used was the TOPKAT ® system (Health Designs, Inc., Rochester, NY). (Enslein, K. Pharm. Rev. 36 (2): 131S-135S, 1984.
4. The suggested interim values are submitted for comment to the Working Group and also to selected individuals in the USEPA.
5. POC for this action are Howard T. Bausum, 410-436-5063, and the undersigned, 410-436-3980.

Glenn J. Leach  
Program Manager  
Health Effects Research  
USACHPPM

**SUGGESTED INTERIM ESTIMATES OF THE REFERENCE DOSE (RfD)  
AND REFERENCE CONCENTRATION (RfC) FOR CERTAIN KEY BREAKDOWN PRODUCTS  
OF CHEMICAL AGENTS**

*Report to the USACHPPM Chemical Standards Working Group*

10 December 1998

Howard T. Bausum, Gunda Reddy and Glenn J. Leach  
Health Effects Research Program, Directorate of Toxicology  
U.S. Army Center for Health Promotion and Preventive Medicine

**Suggested Interim Estimates of the Reference Dose (RfD) and  
Reference Concentration (RfC) for Certain Key Breakdown Products of Chemical Agents  
to the USACHPPM Chemical Standards Working Group**

### Introduction

There is a need for estimates of the oral Reference Dose (RfD) for certain chemical agent products. The compounds of interest are key environmental breakdown products, associated with chemical agents, which may have to be sampled for in soil and water for purposes of human health and ecological risk assessment. Estimates of the RfD will be of use in making decisions regarding cleanup levels for polluted sites or following any unexpected spill event, and in developing detoxification processes for agents and agent-containing munitions. The present agent demilitarization program has heightened the need for such information.

In this report we seek to identify the best estimate of the RfD for the following important and prevalent breakdown products: thiodiglycol (TDG), methyl phosphonic acid (MPA), ethyl methyl phosphonic acid (EMPA), EA2192, and Lewisite oxide, taken together with its hydrated form, 2-chlorovinyl arsonous acid (CVAA). Some basic information about each of these, including the molecular structure and the chemical agent with which it is associated, is given in Table 1. Carcinogenicity is not considered to be a likely problem with any of these, although there is little information on this at present.

The toxicology database on most of these substances is quite limited. This has required conservative or safe-sided estimates, leading in some cases to reasoning from a structurally-related compound, and in others to estimation of RfD based on Quantitative Structure-Activity Relationships (QSAR).

Methods used by the USEPA for derivation of inhalation Reference Concentrations (RfCs) are similar in concept to those used for oral RfDs. Although RfC is a concentration, while RfD is a dose level, both are derived from NOAELs by applying uncertainty factors. The actual analysis of inhalation exposure is, however, more complex than that for oral exposure. In this report suggested RfCs are derived by direct calculation from the suggested RfD and are intended to serve as screening levels only.

### Methods

In suggesting the best possible estimate of RfD for each compound, a chronic or subchronic NOAEL or LOAEL is given first preference, the RfD being then developed using an uncertainty factor (UF) chosen according to USEPA criteria. An experimentally determined chronic or subchronic NOAEL or LOAEL was not found for any of the compounds dealt with in this report, except for TDG.

If a NOAEL or LOAEL is not available, an estimate of the rat chronic LOAEL, derived from Quantitative Structure-Activity Relationships (QSAR) was the next choice. This was done for TDG and MPA, using the commercially-available software system TOPKAT ® (reference 1). In this case a UF was also developed, following USEPA criteria where possible.

For some compounds neither an experimentally determined value nor a QSAR estimate for subchronic or chronic toxicity was available. In these cases, a RfD was derived using data from a structurally related compound of comparable

toxicity. Thus, in the case of EMPA, a RfD estimate was derived using an experimentally-derived rat subchronic NOAEL for isopropyl methylphosphonic acid (IMPA). Similarly, an estimate for lewisite oxide was made using an experimental rat subchronic NOAEL value for Lewisite, while LOAEL values for VX were used as surrogates for the related structure EA2192.

Suggested RfCs were derived by calculation from the calculated RfDs as described above. Where RfC were not available from either the Integrated Risk Information System (IRIS, USEPA) or the Health Effects Assessment Summary Tables (HEAST, USEPA) the RfC values were derived by multiplying the suggested chronic oral RfD (in mg/kg/day) by 70 kg (average body weight of an adult), then dividing by 20 m<sup>3</sup>/day (average adult inhalation rate) and finally multiplying by 1000 to derive a value in microgram/m<sup>3</sup> (references 2,3,4). Thus we employed the following equation to extrapolate oral RfDs to RfCs.

$$\text{RfC} = \frac{\text{RfD} \times 70 \text{ kg}}{20 \text{ m}^3 \times \text{UF}} \times 1000$$

where:

RfC- Inhalation Reference Concentration, micrograms/m<sup>3</sup>

RfD- Reference Dose, mg/kg/day

70kg- Average body weight of an adult, kilograms

20m<sup>3</sup>- Average adult inhalation rate, meter<sup>3</sup>

UF- Uncertainty Factor of three {3} to allow for the uncertainty of extrapolation from an oral to an inhalation route of exposure

#### Development of Reference Dose

**Thiodiglycol:** For this substance an oral LD<sub>50</sub> of 6610 mg/kg was determined in rats (reference 5), indicating rather low toxicity. Estimates using TOPKAT QSAR included 2700 mg/kg for rat oral LD<sub>50</sub>, in fair agreement with the experimental figure (reference 6). The QSAR estimate for rat chronic LOAEL is 1700 mg/kg/day. No evidence for carcinogenicity was found, and the QSAR estimate for this was negative in all of three rodent models.

One provisional estimate of the RfD can be made by use of the QSAR-estimated LOAEL, 1700 mg/kg/day. The safety factor to be applied, i.e., the Uncertainty Factor (UF), should allow a factor of ten for extrapolation from animal study to man, a factor of ten to provide for variation in sensitivity within human populations, a factor of ten for use of a LOAEL instead of NOAEL, and at least a factor of three for use of a QSAR estimate as opposed to experimental data. The UF is then developed as follows:

$$\begin{aligned} \text{UF1} &= 10 \quad (\text{Extrapolation from an animal study to man (interspecies)}) \\ \text{UF2} &= 10 \quad (\text{Human (intraspecies) variability (sensitive subpopulations)}) \\ \text{UF3} &= 10 \quad (\text{Extrapolation from LOAEL to NOAEL}) \\ \text{UF4} &= 3 \quad (\text{Database uncertainties: lack of reproductive and genotoxicity studies}) \end{aligned}$$

The uncertainty factor is then:

$$\text{UF} = 10 \times 10 \times 10 \times 3 = 3,000$$

The estimate is also adjusted by use of a Modifying Factor (MF) which in this case allows for the use of a QSAR



prediction as a basis for RfD derivation. A MF of 3 is assigned.

$$\text{MF} = 3$$

The RfD is derived according to the equation:

$$\text{RfD} = \frac{\text{LOAEL}}{\text{UF} \times \text{MF}} = \frac{1700 \text{ mg/kg/day}}{3000 \times 3} = 0.17 \text{ mg/kg/day} = 170 \text{ ug/kg/day}$$

All RfD estimates, together with essential information about their derivation, are summarized in Table 2.

An alternative estimate of the RfD for this compound can be derived from our ongoing toxicity evaluation of TDG in rats. A 14-day study was conducted in which neat TDG was administered by oral gavage to male and female rats (six/group/sex) at doses of 0, 157, 313, 625, 1250, 2500, and 5000 mg/kg BW/day (5 days/week) (reference 7). No clinical signs or gross morphological changes were noticed in either sex. At the highest dose level, changes in food consumption, and body and kidney weights were observed. Some clinical chemistry parameters were affected at the two highest doses, 2500 and 5000 mg/kg/day. A drop in WBC was seen at higher doses (1250 and 2500) but not at the highest dose, 5000 mg/kg/day.

The 1250 mg/kg/day level was determined to be a NOAEL level. This is suggested by the absence of clinical chemistry, body weight, or organ weight changes, and that the one hematological effect, lowered WBC, was not dose dependent. Histopathology information was not included, but effects at 1250 mg/kg/day are considered unlikely in the light of the body and organ weight results.

The UF is developed as follows:

- UF1 = 10 (Use of an animal study)
- UF2 = 10 (Human variability)
- UF3 = 3 (Database uncertainties: lack of developmental and reproductive studies)
- UF4 = 10 (Extrapolation from subchronic to chronic)

The Uncertainty Factor is then:

$$\text{UF} = 10 \times 10 \times 3 \times 10 = 3,000$$

Modifying Factor (for extrapolation from 14 day to subchronic study)

$$\text{MF} = 3$$

The RfD estimate is then:

$$\text{RfD} = \frac{1250 \text{ mg/kg/day}}{3,000 \times 3} = 0.13 \text{ mg/kg/day} = 130 \text{ ug/kg/day}$$

Thus the RfD, as determined on the basis of the NOAEL from a 14- day study agrees quite well with the value derived from the QSAR estimate of the rat chronic LOAEL: 130 ug/kg/day compared to 170 ug/kg/day.

#### Preferred Derivation:

In a recent subchronic study (rat, 90 day), a NOAEL of 500 mg/ kg/ day was determined (reference 7). This value, because it is based on an experimental result from a subchronic test, will be used here. The MF of 3 for extrapolation

from 14 day to subchronic duration is therefore dispensed with.

$$\text{RfD} = \frac{500 \text{ mg/kg/day}}{3,000} = 0.17 \text{ mg/kg/day} = 170 \text{ ug/kg/day}$$

**Methylphosphonic Acid:** The three compounds MPA, IMPA, and diisopropyl methylphosphonic acid (DIMP) seem to be of very similar toxicity. Thus, for IMPA, the rat subchronic NOAEL was experimentally determined to be 279 mg/kg/day (reference 8), while the rat chronic LOAEL was estimated by TOPKAT to be 221 mg/kg/day (6). For DIMP the rat LD<sub>50</sub> was experimentally determined to be 826 mg/kg (9). A LOAEL of 330 mg/kg/day and NOAEL of 56.5 mg/kg/day were determined for DIMP using mink as the experimental animal (reference 10). For MPA, an experimental LD<sub>50</sub> of 5000 mg/kg was reported (reference 11). The TOPKAT estimate for rat chronic LOAEL is 566 mg/kg/day. Experimental values for this were not found; therefore in this report the QSAR estimate for rat chronic LOAEL will be used.

$$\text{QSAR estimate of rat chronic LOAEL} = 566 \text{ mg/kg/day}$$

The UF is derived as follows.

$$\begin{aligned} \text{UF1} &= 10 \quad (\text{Extrapolation from an animal study}) \\ \text{UF2} &= 10 \quad (\text{Individual/ subgroup variation}) \\ \text{UF3} &= 10 \quad (\text{Extrapolation from LOAEL to NOAEL}) \\ \text{UF4} &= 3 \quad (\text{Use of a QSAR estimate}) \end{aligned}$$

The Uncertainty Factor is then:

$$\text{UF} = 10 \times 10 \times 10 \times 3 = 3000$$

$$\text{MF, incomplete data base} = 3$$

The RfD is then:

$$\text{RfD} = \frac{566 \text{ mg/kg/day}}{3000 \times 3} = 0.057 \text{ mg/kg/day} = 57 \text{ ug/kg/day}$$

#### Preferred Derivation:

A provisional RfD for MPA has been suggested in a USEPA issue paper (reference 12), in which the RfD is derived from analogy to isopropyl methylphosphonic acid (IMPA). For this compound, an experimentally determined subchronic NOAEL in the rat has been determined. This, and a RfD value (100ug/kg/day) derived from it using a UF of 3000, have been placed in the USEPA's IRIS database (reference 13). The RfD value suggested for MPA (reference 12) is based on a total UF of 10,000 and includes an adjustment factor for the ratio of the molecular weight of MPA to that of IMPA. The suggested RfD value for MPA is then 0.02 mg/kg/day (=20 ug/kg/day).

**Ethyl Methylphosphonic Acid and Isopropyl methylphosphonic acid:** The only EMPA data point available is a QSAR estimate of 65 mg/kg for the rat oral LD<sub>50</sub> (reference 6). This suggests a toxicity somewhat greater than that of MPA, but there is no confirmation of this. The approach taken in developing a provisional RfD for EMPA is to use data from the structurally related compound IMPA, for which a RfD has been developed and placed in USEPA's IRIS database (reference 13). In this approach the experimentally-determined subchronic NOAEL (rat) for IMPA, 279 mg/kg/day (reference 8), is used. The UF is derived thus:

For **IMPA**:

UF1 = 10 (Extrapolation from animal study to man)  
 UF2 = 10 (Allowing for sensitive individuals)  
 UF3 = 10 (Subchronic study to chronic)  
 UF4 = 3 (Lack of reproductive or developmental toxicology study or tox study in second species)

The Uncertainty Factor is then:

$$UF = 10 \times 10 \times 10 \times 3 = 3,000$$

The Modifying Factor is:

$$MF = 1$$

$$RfD = \frac{279 \text{ mg/kg/da}}{3000 \times 1} = 0.1 \text{ mg/kg/da} = 100 \text{ ug/kg/da}$$

For **EMPA**:

An additional uncertainty factor of 3 is applied for use of a structurally related compound

$$RfD = \frac{0.1 \text{ mg/kg/da}}{3} = 0.028 \text{ mg/kg/da} = 28 \text{ ug/kg/day}$$

This value introduces the uncertainty of reasoning from a structurally-related compound. However, limited information suggests that IMPA and EMPA are quite similar in toxicity. The estimate is probably reliable, especially in view of the large UF employed in its derivation.

**EA 2192:** There are scant toxicology data on this compound, though a dermal study in rabbits suggests an acute toxicity only somewhat less than that of the parent VX, perhaps less than an order of magnitude (reference 14). Studies of toxicity changes during hydrolysis of VX show a decrease in toxicity (cholinesterase inhibition), but the fall in toxicity does not keep pace with the disappearance of VX. This indicates that the toxic hydrolysis product EA2192 possesses a toxicity that is lower, but comparable, to that of the parent VX (reference 15). Toxicity estimates using the TOPKAT QSAR system gave unreliable results (reference 6), and these cannot be used in estimation of a RfD.

Because of the similarity to VX, as well as the lack of useful data or useful QSAR estimates, the experimental toxicity values available for VX will be used as a surrogate for EA2192. In deriving an estimate of the RfD for the related EA2192, a factor of ten for use of a related compound will not be necessary, because VX is considered to be at least as toxic as EA2192.

There is currently no RfD for VX published in the IRIS database. An interim RfD has been published by the Army Surgeon's Office and is currently being reviewed by the National Academy of Sciences/ NRC SubCommittee on Chronic Reference Doses for Selected Chemical Warfare Agents (reference 16). The interim RfD is 0.0006 ug/kg/day, and was derived from a LOAEL of 0.06 ug/kg/day determined on the basis of whole blood cholinesterase inhibition in sheep.

**Lewisite Oxide:** The hydrolysis of Lewisite (2-chlorovinyl dichloroarsine) yields 2-chlorovinyl arsonous acid (CVAA). This loses water to form 2-chlorovinyl arsenous oxide (Lewisite oxide), but this can be quantitatively reversed when the oxide is dissolved in water, or the oxide and the dibasic acid may exist in equilibrium (references 17, 18). Lewisite is considered more toxic than its hydrolysis product and lewisite oxide; however the hydrolysis product retains the trivalent arsenic and much of the toxicity of Lewisite (references 5,19).

For Lewisite oxide, and its hydration product, the RfD developed for Lewisite is suggested as a surrogate. This value is also currently under review by the National Academy of Sciences NRC Committee on Chronic Reference Doses for Selected Chemical Warfare Agents. The proposed RfD is 0.1 ug/kg/day. The RfD for Lewisite was derived from a NOAEL of 0.6 mg/kg/day (time-adjusted to 0.44mg/kg/day) determined in a multi-generational study in rats.

#### Calculation of Reference Concentration (RfC)

Since there are no inhalation toxicity data on the chemical breakdown products listed in Table 1, The suggested RfC is derived in each case from the RfD calculated above and listed in Table 2. The RfC, calculated as described under Methods, are listed in Table 3, together with the RfD values.

#### Discussion

In this study, several compounds lacked both laboratory data and QSAR estimates that might serve as starting points for development of provisional RfD values. For each of these compounds, EMPA, EA2192, and lewisite oxide (2-chlorovinyl arsenous oxide), the RfD was estimated using data relating to a closely related, surrogate compound. In each case it is unlikely that the surrogate compound is significantly less toxic than the compound of interest.

In the case of lewisite oxide/ chlorovinylarsonous acid, the use of TOPKAT is not possible because currently available models do not cover metalo-organics. The QSAR estimates for EA2192 and for rat chronic LOAEL in the case of EMPA were not usable because of the 'location' of these molecular structure far outside of the 'optimum prediction space' of the pertinent TOPKAT models.

Usable QSAR estimates were available only for TDG and MPA. In these cases, RfD were estimated on this basis, while for TDG an additional estimate was made from a short term experimental NOAEL value. These two estimates differed by less than a factor of two.

In cases where neither usable laboratory-derived values nor acceptable QSAR estimates are available for chronic or subchronic LOAEL or NOAEL, a short-term or acute toxicity value, such as an LD<sub>50</sub> may be the only or best endpoint available for the particular compound. The problem of estimating RfD from LD<sub>50</sub> was studied by Layton *et al.*, 1987 (18) who analyzed data from a large number of compounds. Their study suggests that, although not a substitute for subchronic or chronic toxicity data, the LD<sub>50</sub> (mg/kg) can be used to estimate the RfD by multiplying by a factor of  $5 \times 10^{-6}$  to  $1 \times 10^{-5}$ . This approach introduces much uncertainty, because of the wide variability of the ratio LD<sub>50</sub>/RfD and the possibility that acute and chronic effects may arise through different mechanisms. Derivation from LD<sub>50</sub> was not used in this study, with the use of a suitable surrogate compound being given preference.

The methods EPA uses in derivation of Reference Concentrations (RfC) are similar in concept to those used for oral RfDs; however, the actual analysis of inhalation exposure is more complex than for oral exposure. This is due to the dynamics of the respiratory system and its diversity across the species and to differences in the physicochemical properties of contaminants. RfCs are derived from NOAELs by applying uncertainty factors similar to those used for oral RfDs as well as appropriate factors for respiratory volume and other factors. The inhalation values derived from oral RfDs are intended to serve as screening levels only. Thus they do not represent EPA guidance (references 2,4).

#### Summary:

Provisional estimates of Reference Dose (RfD) have been made for five key breakdown products of chemical warfare agents, viz., thiodiglycol (TDG), methyl phosphonic acid, (MPA), ethyl methyl phosphonic acid (EMPA), EA 2192, and lewisite oxide/2-chlorovinyl arsonous acid. The chemicals are identified in Table 1, while the RfD values, with other essential information, are given in Table 2. Laboratory data, apart from acute toxicity information, that was usable for RfD development was available only for TDG. Usable QSAR estimates (of rat chronic LOAEL) were available only for TDG and MPA. For TDG, both the experimental and the QSAR information were used.

For the remaining compounds, EMPA, EA2192, CVAA and Lewisite oxide, information and existing or proposed RfD values from surrogate, closely related compounds were used. For EMPA the existing RfD for isopropyl methyl phosphonic acid (IMPA), currently listed in USEPA's IRIS database, was used as a surrogate. For EA2192, CVAA, and Lewisite oxide, currently proposed RfD's for VX and Lewisite, respectively, are listed. These, when accepted, are probably the best values for these two hydrolysis products.

Suggested inhalation Reference Concentration (RfC) values were calculated from the calculated RfD values. These values are intended for screening purposes only.

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**TABLE 1: Selected Key Breakdown Products of Chemical Agents**

<u>Substance</u>	<u>CAS No.</u>	<u>Name</u>	<u>Product of</u>	<u>Structure</u>
TDG	111-48-8	Thiodiglycol	Sulfur mustard	$\text{HO-CH}_2\text{-CH}_2\text{-S-CH}_2\text{-CH}_2\text{-OH}$
MPA	993-13-5	Methyl-phosphonic acid	GB, VX	$\text{CH}_3\text{-P(OH)(OH)=O}$
EMPA	1832-53-7	Ethyl methyl-phosphonic acid	VX	$\text{CH}_3\text{-CH}_2\text{-O-P(OH)(CH}_3\text{)=O}$
IMPA	1832-54-8	Isopropyl methyl-phosphonic acid	GB	$(\text{CH}_3)_2\text{CH-O-P(OH)(CH}_3\text{)=O}$
EA 2192	73207-98-4	S-(2-diisopropylaminoethyl) methylphosphonothioic acid	VX	$((\text{CH}_3)_2\text{CH})_2\text{N-CH}_2\text{CH}_2\text{S-P(OH)(CH}_3\text{)=O}$
Lewisite oxide	3088-37-7	2-chlorovinyl arsenous oxide	Lewisite	$\text{Cl-CH=CH-As=O}$
CVAA	85090-33-1	2-chlorovinyl arsonous acid	Lewisite	$\text{Cl-CH=CH-As(OH)}_2$



**TABLE 2: Summary of Estimates of Reference Dose for Products of Chemical Agents**

<u>Chemical</u>	<u>Basis for Derivation of RfD/ RfC</u>	<u>Safety Factor</u>	<u>mg/kg/da</u>	<u>ug/kg/da</u>
<b>TDG</b>	LOAEL (rat, chronic, QSAR est.) = 1700 mg/kg/da (Ref. 6)	UF = 3000 MF = 3	0.17	170
	14 da NOAEL, rat = 1250 mg/kg/da (Ref. 7)	UF = 3000 MF = 3	0.13	130
	<b>90 da NOAEL, rat = = 500 mg/kg/da (Ref. 7)</b>	<b>UF = 3000 MF = 1</b>	<b>0.17</b>	<b>170</b>
<b>MPA</b>	LOAEL (rat, chronic, QSAR est.) = 566 mg/kg/da (Ref. 6)	UF = 3000 MF = 3	0.057	57
	<b>NOAEL, for IMPA (rat, subchronic) = 279 mg/kg/da (Ref. 12*)</b>	<b>UF = 10000 MF = 1</b>	<b>0.02</b>	<b>20</b>
<b>* includes adjustment for MW MPA/IMPA)</b>				
<b>EMPA</b>	<b>NOAEL, for IMPA (rat, subchronic) = 279 mg/kg/da (Ref 12)</b>	<b>UF = 3000 MF = 3</b>	<b>0.028</b>	<b>28</b>
<b>IMPA</b>	<b>NOAEL = 279 = 279 mg/kg/day (Ref. 12)</b>	<b>UF = 3000 MF = 1</b>	<b>0.1</b>	<b>100</b>
<b>EA 2192</b>	<b>LOAEL for VX (sheep, subchronic, Based on ChE inhibition) = 0.06 ug/kg/da</b>	<b>UF = 90 MF = 1</b>	<b>6 E-7</b>	<b>0.0006</b>
<b>Lewisite oxide/CVAA</b>	<b>Time-adjusted NOAEL for lewisite (rat, subchronic) = 0.44 mg/kg/da</b>	<b>UF = 3,000 MF = 1</b>	<b>0.0001</b>	<b>0.1</b>

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**BOLDED values represent the preferred estimate**

**TABLE 3. Estimated Reference Concentration (RfC) Values and Corresponding RfD Values.**

Compound	RfD ☆ (mg/kg/da)	RfC ★ (µg/m <sup>3</sup> )
TDG	0.17	200
MPA	0.020	24
EMPA	0.028	34
IMPA	0.100	110
EA 2192	0.0000006	0.0007
Lewisite oxide/ CVAA	0.0001	0.11

—  
☆ Values from Table 2, q.v. for derivation.

★ Derived from RfD Values as described under Methods.

## APPENDIX F - ANNEX F.2

FROM: MCHB-TS-THE

25 Jan, 1999

TO: MCHB-TS-EHRARC, (Attn: Ms. Veronique Hauschild)

SUBJECT: Status of the request to review the oral RfD for the VX hydrolysis product EA2192.


1. General

a) The oral RfD for EA2192 is now set at the same level as that of VX. This is believed to be overprotective because the ionized state of the EA2192 molecule limits its absorption. All dermal absorption and the majority of the compounds sorbed via the oral route are taken up by passive absorption. High polarity diminishes this uptake and ionization such as is seen with EA 2192 strongly inhibits this process. Dermal studies performed with EA2192 have demonstrated that this compound is excluded by the skin to such an extent that no effects were seen at any of the test dosages used. A comparison of the oral LD50 values for VX and EA2192 reveals a similar situation. The oral LD50 for VX is 12 µg/Kg while the oral LD50 for EA2192 is 630 µg/Kg.

b) Despite the above comparisons and the 50 fold higher LD50 of EA2192 we can not recommend a higher RfD at this time. The reason for our decision is that the limited information on the chronic toxicity of this compound. Considerable uncertainty exists as to the mechanism of the chronic toxicity of phosphonate nerve agents at very low doses. Recent evidence suggests that chronic toxicity of organophosphorus compounds may not be totally due to their action on AChE. Moreover, the studies reported by Michel et al. seem to demonstrate the AChE toxicity caused by EA2192 may be more refractory to nerve agent antidote treatment than toxicity induced from other agents. Although the response of a toxicant to an antidote is not considered in establishment of a RfD this evidence provides an indication that the complex formed between EA2192 and AChE may have greater stability than the complex with VX. Because RfD values are designed to provide protection during chronic exposures, it is important to distinguish between chronic and acute effects. Increases in the long term stability of the phosphonate / enzyme complex may have limited effect on acute toxicity but may contribute to higher steady state concentrations of the inactivated enzyme and hence pose a greater potential for chronic toxicity.

2. Time required for this work: 2 hours

3. POC for this review is M. Major, 410-612-7159

  
GLENN J. LEACH  
Program Manager  
Health Effects Research

## APPENDIX G

### TOXICITY OF AGENTS GA AND GD RELATIVE TO THE TOXICITY OF AGENT GB

It was assumed that the relative acute toxicity, expressed as a ratio of the mean LD<sub>50</sub> values, would also apply to minimum effect levels (MELs). The LD<sub>50</sub> values for monkeys and rats for all three agents are given in Table G-1. Data for all exposure routes were used except for percutaneous studies. The latter were considered inappropriate because effect levels are likely to be substantially affected by environmental test conditions and the volatility of the individual agent. Even though the absolute toxicity of the agents varies from species to species and also from one exposure route to another, the relative toxicity, as expressed by the ratios of the LD<sub>50</sub> values, is expected to be similar because the mechanism of action of all three agents is identical. Where more than one LD<sub>50</sub> value was available for a given species and exposure route, the geometric mean was calculated. The GA/GB and GD/GB ratios for each species were then determined, and the geometric mean for each set of ratios was calculated. The final mean value for GA/GB was 2.65 and the final mean value for GD/GB was 0.63, indicating that in terms of acute toxicity GA is less than half as toxic as GB and GD is about twice as toxic as GB. These ratios are similar to those derived from comparing the potency of the agents to inhibit acetylcholinesterase. The pI<sub>50</sub> values (negative log of the concentration causing 50% AChE? inhibition), for GA, GB, and GD are 8.6, 8.9, and 9.2 (Dacre, 1984), equivalent to  $2.5 \times 10^{-9}$ ,  $1.26 \times 10^{-9}$ , and  $6.3 \times 10^{-10}$  mol/L, respectively. The GA/GB and GD/GB ratios are 1.99 and 0.5, very similar to those derived from the acute lethality data.

Therefore, to estimate the MELs:

$$\text{MEL of GA} = 2.65 \times \text{MEL of GB}$$

$$\text{MEL of GD} = 0.63 \times \text{MEL of GB}$$

Table G-1. Estimate of the Toxicity of GA and GD Relative to GB

Route	Species	LD <sub>50</sub> Values (µg/kg)				Ratio of Effect		References		
		GB	GA	GD		GA/GB	GD/GB	GB	GA	GD
Inhal.	monkey	74 <sup>a</sup>	187 <sup>a</sup>	-	-	2.53	-	DA, 1974	DA, 1974	-
	rat	220 <sup>a</sup>	450 <sup>a</sup>	230 <sup>a</sup>	1.05	2.05	1.05	DA, 1974	DA, 1974	DA, 1974
I.V.	monkey	20	~50	-		~2.5		DA, 1974	DA, 1974	DA, 1974
	rat	39	70	50				RTECS, 1997	DA, 1974	DA, 1974
	rat	45		44.5				DA, 1974	DA, 1974	RTECS, 1997
	mean value <sup>b</sup>	42	70	47	1.12	1.67				
Oral	rat	550	3700	400				RTECS, 1995	Grob & Harvey, 1958	DA, 1974
	rat	600						Grob & Harvey, 1958		
	rat	870-1000						DA, 1974		
	mean value <sup>b</sup>	676	3700	400	0.59	5.47				
Subcut.	rat	103-108	162	71				RTECS, 1997	RTECS, 1997	RTECS, 1997
	rat		~300						DA, 1974	
	mean value <sup>b</sup>	106	220	71	0.67	2.07				
I.M.	monkey	22	34	9.5	0.43	1.55		RTECS, 1997	RTECS, 1995	RTECS, 1997
	rat	108	800	62				RTECS, 1997	Grob & Harvey, 1958	RTECS, 1997
	rat	112						DA, 1974		
	rat	170						Grob & Harvey, 1958		
	mean value <sup>b</sup>	127	800	62	0.49	6.30				
I.P.	rat	218	~800	98				RTECS, 1997	DA, 1974	RTECS, 1997
	rat	250	490					DA, 1974	RTECS, 1997	
	mean value <sup>b</sup>	233	626	98	0.42	2.69				
OVERALL MEAN VALUE <sup>c</sup>					2.65					
					0.63					

<sup>a</sup> 10-mi n LC<sub>50</sub> in mg-min/m<sup>3</sup><sup>b</sup> Geometric mean for rat<sup>c</sup> Overall geometric mean for rats and monkeys combined



## APPENDIX H

### DERIVATION OF DERMAL ABSORPTION FACTORS FOR CHEMICAL AGENTS IN SOIL

**MCHB-DC-THE**

**January 20, 1998**

**SUBJECT:** Derivation of Dermal Absorption Estimates for Chemical Warfare Agents

**FROM:** Health Effects Research Program

**MEMORANDA FOR** Acting Program Manager, EHRARC, (Attn: Ms. Veronique Hauschild)

This document reports an estimation of dermal absorption of the chemical warfare (CW) agents HD, GA, GB, GD, VX and L from soil. It is important to note that dermal absorption of Lewisite from soil would be unlikely because it is not stable in water.

1. General Comments: Improvements in our model for calculation of the dermal adsorption of compounds from soil required recalculation of estimate for hourly absorption of chemical warfare agents from soil. Background information on the model is also included.
2. The publication of the EPA's interim report on "Dermal Exposure Assessment: Principles and Applications" in 1992 was a landmark in the area of risk assessment of soil pollutants. That report compiled the very limited experimental data then available, outlined some guidelines about experimental methods and issued the guidance that accurate predictive models would not be possible until a better understanding of the processes involved and more experimental data were available. The response to this guidance in the EPA regions and at the state level was to begin to handle assessment of this risk by adoption of default values for absorption of compounds from soil. The Army now is often required to use default values for absorption of toxic compounds from soil in the range of 3% to 30%.

Default values of this magnitude grossly overestimate dermal absorption from soil for several reasons. These defaults were established by application of large uncertainty factors to the experimental data that was available in the 1992 EPA report. In addition, the studies referenced in that report commonly used 96 hour exposures in rats and freshly prepared soil/pollutant preparations in their experimental method. Such methods overestimate the results in humans because people have lower dermal absorption rates than rats and people exposed to contaminated soils commonly have dermal exposures of much less than 96 hours. Even more importantly, most soils contaminated by Army operations have been acted on by decades of sun and rain, which have reduced the bioavailability of the pollutants they contain. Recent work in Dr. Martin Alexander's Laboratory at Cornell has demonstrated that pollutants present in the soil at low concentration

are, over time, sequestered in the soil matrix and pore water with concomitant losses in toxicity. These studies show that weathering of soil/pollutant mixtures commonly produces reductions in toxicity from 60 to 100%. This phenomenon is seen even in sterilized soils where metabolism and biological binding processes are absent. It is characteristic of such processes that the sequestered compounds can be recovered quantitatively with modern analytical procedures.

It is also important to note, that the data referenced in the 1992 EPA report were predominately from studies with large, halogenated, hydrophobic compounds having extremely limited aqueous solubility. Chemical warfare agents and most other Army contaminants of concern are smaller, more volatile, and more hydrophilic. It is generally accepted that dermal absorption of an organic compound increases with the octanol/water partition coefficient (Kow), and this value is a function of hydrophobicity. The chemicals used in the USEPA report all had very large Kow values compared to those of the CW agents.

#### Kow VALUES FOR USEPA COMPOUNDS

- |                                     |                  |
|-------------------------------------|------------------|
| 1. Hexadecane = $> 1.0 \times 10^7$ | (log Kow $> 7$ ) |
| 2. TCDD = $6.31 \times 10^6$        | (log Kow 6. 8)   |
| 3. TCB = $5.0 \times 10^5$          | (log Kow 5.7)    |
| 4. DDT = $9.5 \times 10^5$          | (log Kow 5.98)   |

#### Kow VALUES FOR CW AGENTS

- |                                      |                   |
|--------------------------------------|-------------------|
| 1. GB Kow = 1.99                     | (log Kow = 0.299) |
| 2. GA Kow = 2.42                     | (log Kow = 0.38)  |
| 3. GD Kow = 66.6                     | (log Kow = 1.82)  |
| 4. VX Kow = 123                      | (log Kow = 2.09)  |
| 5. HD Kow = 23.4                     | (log Kow = 1.37)  |
| 6. 2-chlorovinylarsonous acid = 0.85 | (log Kow = -0.07) |

Notes: The Kow of Lewisite cannot be determined since this compound is not stable in water. ARMY FM 3-9 reports that "The rate of hydrolysis is rapid for both vapor and dissolved Lewisite and when the humidity is high Lewisite hydrolyzed so rapidly that it is difficult to maintain a concentration sufficient to blister even unprotected skin." Lewisite oxide is the species formed when Lewisite is hydrolyzed and then dried. It is, in turn, converted quantitatively to 2-chlorovinylarsonous acid when dissolved in water. The latter compound represents the Lewisite species actually found in water.

The values given for the log Kow of HD and G-agents (MRICD 1998) are experimentally determined; the value for VX is calculated (Britton and Grant, 1988; Small, 1984). The EPA compounds listed all have very low vapor pressure and would not tend to evaporate from the skin prior to absorption. The G-agents, however, all have rather high vapor pressures. Indeed, GB evaporates at a rate similar to water.



It becomes clear that accurate prediction of the dermal absorption of CW agents will require a new approach. The magnitude of the exposure must be calculated as a function of the predicted duration of the exposure rather than using data from 96 hour studies and the model must predict sorption from the physical and chemical properties of the individual compounds and from the soils at the site of the contamination.

In developing a new model for prediction of any behavior, selection of a narrow range of conditions so that one process predominates and competing processes can be safely ignored tends to simplify and increase the accuracy of the estimation process. To do this, we have limited our studies to more water soluble compounds and defined our exposure times as 12 hours or less. Imposition of these limits tends to ensure that the principal route of percutaneous transport will be by dissolution of the compounds in water. In such a system, the pollutants leave the soil and are introduced to the skin by the aqueous route. It is well established that the partition of a compound between soil and water ( $K_{sw}$ ) can usually be described by calculation of the theoretical partition of the compound between organic carbon and water ( $K_{oc}$  = mg/g of organic carbon (in soil)/mg per mL in solution) and then correcting this value for the fractional concentration of organic carbon in the soil ( $f_{oc}$ ).

$$K_{sw} = K_{oc} \times f_{oc}$$

The most accurate calculation of soil adsorption coefficients for compounds with properties like the CW agents is a simple linear regression using  $K_{ow}$  for the independent variable (Lyman et al., 1982).

$$\log K_{oc} = 0.544 \log K_{ow} + 1.377$$

Thus,  $K_{oc}$  values for the CW agents:

GB  $K_{oc}$  = 34.6

GA  $K_{oc}$  = 38.5

GD  $K_{oc}$  = 234

VX  $K_{oc}$  = 327

HD  $K_{oc}$  = 133

It has also been shown that the rate of penetration (flux) of a compound through the skin relates in a positive fashion to the compound's water solubility (WS) and octanol/water partition coefficient ( $K_{ow}$ ) and inversely to its molecular weight (MW). Numerous formulas are available to predict this behavior. The formula of Fiserova-Bergerova et al. (1990) shows particular promise in the prediction of the dermal absorption of compounds of moderate solubility in water.

$$\text{Hourly flux} = 0.067WS (0.038 + 0.153 K_{ow}) e^{-0.016MW}$$

FL = Flux (penetration through the skin)

WS = water solubility

Kow = octanol/water partition

MW = molecular weight

The molecular weights (MW) and water solubilities (WS) of the CW agents are:

GB MW = 140.1; WS = miscible (1 g/mL used as default)

GA MW = 162.1; WS = 98 mg/mL

GD MW = 182.2; WS = 21 mg/mL

VX MW = 267.4; WS = 30 mg/mL

HD MW = 159.1; WS = 0.92 mg/mL

Therefore, FL values for the CW agents (given in terms of the amount of agent that will penetrate a square cm of skin in one hour) can be calculated.

GB FL = 2.41 mg/cm<sup>2</sup>

GA FL = 0.20 mg/cm<sup>2</sup>

GD FL = 0.78 mg/cm<sup>2</sup>

VX FL = 0.53 mg/cm<sup>2</sup>

HD FL = 1.31 mg/cm<sup>2</sup>

In order to link the concepts of soil/water partition and hourly flux together into a model to predict dermal uptake from soil, it is necessary to follow the fate of a quantity of compound through these processes. It is probably not true that one mL of water will obtain equilibrium with one gram of soil; the equilibrium would most certainly be between one mL of water and much less than a gram of soil. However, we will use the one gram number as one means of safe siding this model. It is also inaccurate to assume that soil/water equilibrium will occur more or less instantaneously but we will also make this assumption. Thus, the concentration of pollutant in the soil (mg/g) divided by the  $K_{sw}$  yields the concentration of pollutant in water (mg/mL). If we make the additional assumption that the material moving through 1 cm<sup>2</sup> of skin in one hour is drawn exclusively from this volume (1 mL will form a layer of water over 1 cm<sup>2</sup> of skin that is 1 cm deep), then the flux divided by the amount of compound in the 1 mL of water becomes the fractional absorption in one hour. We can relate these two equations to obtain a formula for calculation of percent absorption from soil per hour.

$$\text{Percent of soil contaminant absorbed/hour} = \text{hourly flux/WS} \times 100 (1/K_{sw})$$

Using this formula and the chemical-specific FL, WS, and K<sub>sw</sub> values given above, the hourly dermal absorption rates for the CW agents were calculated for a soil with 2% organic carbon.

**Hourly dermal absorption of CW agents from soil of 2% organic carbon:**

**GB = 0.35%**

**GA = 0.26%**

**GD = 0.78%**

**VX = 0.27%**

**HD = 0.70%**

## Conclusions

1) Sequestration of pollutants in weathered soil makes accurate experimental determination of K<sub>sw</sub> difficult because the soil/water partition can take months to establish. This process also limits the concentration of toxicants transferred from weathered soils to water during the limited time frames that are characteristic of dermal exposures. Because this model assumes rapid and complete equilibrium between soil and water it will usually overestimate values of hourly flux. Comparison of calculated results with experimental results confirms this contention. Experimental values for dermal absorption of TNT, TNB, RDX, and thiodiglycol, performed with an *in vitro* pig skin system using two different soils, indicate that the model normally overestimates absorption on the order of 2 to 2.5 fold. Similar results were seen *in vivo* in primate studies of absorption of 2,4D from soil. Due to the moderate molecular weight and aqueous solubility of the chemical warfare agents, this model should predict their dermal absorption with good accuracy. However, the blister agent HD will have a much lower dermal transport than predicted because of its reactivity with the skin and its very rapid rate of hydrolysis in aqueous environments (half life is about 4 minutes at body temperature).

2) This is the only model known to this author that has demonstrated accuracy in prediction of the dermal absorption of military significant compounds from soil. USACHPPM is currently seeking acceptance of this model as a predictive tool for risk assessment at military installations. The model has been presented to the EPA's Office of Risk Assessment and will be presented to the risk assessment activity of the Office of The Superfund in Feb. 1998. Use of this model rather than reliance on default values will greatly improve the accuracy of the assessment process and may achieve significant reductions in cleanup costs at military installations.

3) This model uses a minimum default value of 2% organic carbon in the soil. This is because for the purposes of predicting a soil/water partition coefficient, soil has other properties than organic carbon that contribute to the soil/water partition. At high organic carbon concentrations these other properties have a negligible effect on the partition but at low organic carbon concentrations they become more significant.

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